



2015 International Chemical Congress of Pacific Basin Societies

DECEMBER 15–20, 2015 • HONOLULU, HAWAII



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PACIFICHEM 2015 CHAIRMAN'S WELCOME

Welcome and warmest Aloha! On behalf of Pacifichem, Inc., the American Chemical Society, the Chemical Society of Japan, the Canadian Society for Chemistry, the New Zealand Institute of Chemistry, the Royal Australian Institute of Chemistry, the Korean Chemical Society and the Chinese Chemical Society, it is my great pleasure to welcome all of the participants and their guests to the 2015 International Chemical Congress of Pacific Basin Societies - Pacifichem 2015. This is the seventh in this distinguished series of chemistry-related meetings traditionally held in December in Honolulu.

The theme of Pacifichem 2015 is ***Networking – Building Bridges across the Pacific***. As with all past Pacifichem congresses, Pacifichem 2015 fosters collaborations among Pacific Basin chemical scientists to improve the quality of life throughout the world. The venue is Honolulu, on the beautiful island of Oahu, which is located in the central Pacific Ocean, around which two-thirds of the world's population lives. Since the first Congress in 1984, this conference has seen tremendous growth. Over 18,000 papers were submitted for this year's meeting. There are 334 symposia and a total of 1,493 oral and poster sessions. The outstanding technical program truly represents collaborations among Pacific Rim scientists. Each symposium has organizers from at least three different Pacific Rim countries. The technical program represents contributions from 71 countries. The result of such collaborations can only bring improvements in technical development and a better quality of life for all people.

There is much to do on this beautiful island, both independently and as part of the Pacifichem program. I hope you will be able to join us for the Pacifichem Opening Ceremony. This begins with a traditional Hawaiian Chant, followed by the Pacifichem Lecture. Sam Kean, the New York Times bestselling author of *The Disappearing Spoon*, is the Pacifichem Plenary Lecturer. The Periodic Table is one of our crowning scientific achievements, but it's also a treasure trove of passion, adventure, betrayal, and obsession. *The Disappearing Spoon* delves into every single element on the table and explains each one's role in science, money, mythology, war, the arts, medicine, alchemy, and other areas of human history, from the Big Bang through the end of time. His stories have appeared in *The Atlantic Monthly*, *The New York Times Magazine*, *Psychology Today*, *Mental Floss*, and *Slate*, and his work has been featured on NPR's "Radiolab," "All Things Considered," and "Fresh Air."

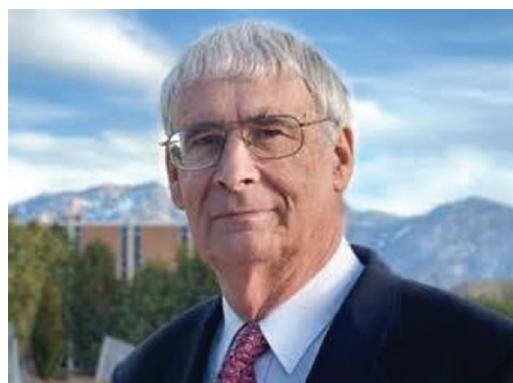
All of the members and staff on the Pacifichem 2015 Organizing Committee have spent many hours preparing for this Congress to make it the best possible. We are excited about the outcome and hope that you will find this Congress fruitful, enjoyable and worthwhile. Mahalo.

Peter Stang is the chair of Pacifichem 2015. He is a Distinguished Professor of Chemistry at The University of Utah and has been the editor of the Journal of the American Chemical Society since 2002. He holds a B.S. from DePaul University and a Ph.D. from the University of California, Berkeley.

Working with chemical systems built from molecular components, Stang has advanced organic chemistry for five decades. He and his team are molecular architects who rearrange the building blocks of chemistry to create new and better products to serve advanced medicine, information storage, and energy.

In recognition of his achievements as a pioneer in supramolecular chemistry, Stang received the National Medal of Science in 2011, followed by the American Chemical Society's (ACS) 2013 Priestley Medal. His major scientific contributions began in the late 1960s with his synthesis of vinyl trifluoromethanesulfonates, which are used to join two completely different hydrocarbons and thus create a chemical reaction. In the 1990s, his synthesis of molecular squares led to the development of several functional, self-assembled chemical systems. Most notably, Stang's method of preparing cyclic structures containing metal-complex units—known as the directional bonding approach—has enabled his team to synthesize elaborate molecules such as tetrahedral frameworks, trigonal prisms and cage-like metallocyclic dodecahedrons. This allows the construction of an intricate molecular framework, ultimately leading to the rapid assembly of nanoscale molecular devices for broad-based, practical applications.

Stang is a member of the American Chemical Society, the American Academy of Arts & Sciences, the National Academy of Sciences, the Chinese Academy of Sciences, and the Hungarian Academy of Sciences. He received the Fred Basolo Medal for Outstanding Research in Inorganic Chemistry in 2009, the Paul G. Gassman Distinguished Service Award of the American Chemical Society's Division of Organic Chemistry, and the F.A. Cotton Medal for Excellence in Chemical Research, in 2010. His research has garnered several other awards from the American Chemical Society, including the ACS Award for Creative Research and Applications of Iodine Chemistry, and the ACS George A. Olah Award in Hydrocarbon or Petroleum Chemistry, the ACS James Flack Norris Award in Physical Organic Chemistry, and the Linus Pauling Medal. He has more than 500 publications and more than 23,500 citations to his credit and has mentored nearly 100 graduate students and postdoctoral fellows.





Proclamation

WHEREAS, the seventh International Chemical Congress of Pacific Basin Societies will convene in Honolulu from December 15–20, 2015, and will host an estimated 16,000 participants, including chemists and chemical engineers, from all over the world; and

WHEREAS, this conference, held every five years, will feature products, services, and publications from a variety of companies during its Pacifichem 2015 Exposition; and

WHEREAS, the 334 symposia focusing on 11 specific scientific areas bring together scientists from all over the world, where the latest research in various fields of chemistry is being conducted; and

WHEREAS, the conference will showcase the knowledge, advancements, and products and services that improve the efficiency of international chemical professionals, local and global environments, and our well-being; and

WHEREAS, the American Chemical Society, Canadian Society for Chemistry, Chemical Society of Japan, New Zealand Institute of Chemistry, Royal Australian Chemical Institute, Korean Chemical Society, and Chinese Chemical Society jointly sponsor this learned gathering, which is one of the largest and most prestigious of international scientific meetings,

NOW, THEREFORE, I, KIRK CALDWELL, Mayor of the City and County of Honolulu, do hereby proclaim December 15–20, 2015, to be

PACIFICHEM 2015 DAYS

in recognition of the outstanding contributions of chemical scientists and to commend the sponsors of this event for hosting this productive international gathering that promotes scientific exchange in the Pacific Basin.

Done this 1st day of December, 2015,
in Honolulu, Hawai‘i.

A handwritten signature in black ink, appearing to read "Kirk Caldwell".

KIRK CALDWELL





Proclamation

Presented to

The 2015 International Chemical Congress of the Pacific Basin Societies

WHEREAS, the seventh International Chemical Congress of Pacific Basin Societies will convene in Honolulu, Hawai'i from December 15 – 20, 2015; and

WHEREAS, the congress, known as Pacifichem 2015, is co-sponsored by the chemical societies of Australia, Canada, China, Japan, Korea, New Zealand, and the United States, with representative from more than 57 other chemical societies headquartered in Pacific nations, who will be among those participating in this important gathering; and

WHEREAS, chemists from more than 71 countries will gather to present more than 17,800 papers and discuss recent discoveries in their fields with the promise of making significant contributions to the science of chemistry and to the general advancement of scientific knowledge; and

WHEREAS, Hawai'i is proud to host Pacifichem 2015, widely recognized as one of the largest and most prestigious international scientific meetings in the world;

THEREFORE I, DAVID Y. IGE, Governor, and I, SHAN S. TSUTSUI, Lieutenant Governor of the State of Hawai'i, do hereby proclaim December 15 – 20, 2015 as

"CHEMISTRY WEEK"

in Hawai'i and encourage the citizens of the Aloha State to join us in welcoming the participants of Pacifichem 2015 to our islands and offering them our best wishes for a memorable conference.

DONE at the State Capitol, in the Executive Chambers, Honolulu, State of Hawai'i, on this twenty-third day of September 2015.

A stylized signature of "David Y. Ige" in black ink.

DAVID Y. IGE
Governor, State of Hawai'i

A stylized signature of "Shan S. Tsutsui" in black ink.

SHAN S. TSUTSUI
Lt. Governor, State of Hawai'i

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OFFICIAL PARTICIPATING ORGANIZATIONS



CO-SPONSORING SOCIETIES

American Chemical Society

Canadian Society for Chemistry

Chemical Society of Japan

Chinese Chemical Society

Korean Chemical Society

New Zealand Institute of Chemistry

The Royal Australian Chemical Institute

OFFICIAL PARTICIPATING ORGANIZATIONS

Australia: Australian Peptide Association

Japan Technical Association of the Pulp and Paper Industry

The Society of Photography and Imaging of Japan

Brunei: Brunei Darussalam Institute of Chemistry

Society of Environmental Science

The Society of Polymer Science, Japan

Canada: Canadian Society for Chemical Engineering

Society of Sea Water Science, Japan

The Society of Rubber Science and Technology

China: Hong Kong Chemical Society

The Electrochemical Society of Japan

The Society of Synthetic Organic Chemistry, Japan

India: Amity Institute for Environmental Toxicology, Safety and Management (AIETSM)

The Fullerenes, Nanotubes and Graphene Research Society

The Surface Finishing Society of Japan

Indonesia: Himpunan Kimia

The Japan Institute of Energy

Malaysia: Institut Kimia Malaysia, Kuala Lumpur

Japan: Catalysis Society of Japan

The Japan Petroleum Institute

Mexico: Sociedad Quimica de Mexico (SQM)

Combustion Society of Japan

The Japan Society for Analytical Chemistry

Nepal: Nepal Chemical Society

Japan Association for International Chemical Information

The Japan Society of Applied Physics

Papua New Guinea: The Institute of Chemists, PNG (ICPNG)

Japan Coating Technology Association

The Japan Wood Research Society

Philippines: Integrated Chemists of the Philippines

Japan Explosives Society

The Japanese Photochemistry Association

Republic of Korea: Korean Society of Radiopharmaceuticals and Molecular Probes (KSRAMP), Korean Society of Water and Wastewater (KSWW)

Japan Oil Chemists' Society

The Japanese Society for Food Science and Technology

Singapore: Singapore National Institute of Chemistry

Japan Society for Bioscience, Biotechnology, and Agrochemistry

The Japanese Society for the History of Chemistry

Sri-Lanka: Institute of Chemistry Ceylon

Japan Society of Electromagnetic Wave Energy Applications (JEMEA)

The Japanese Society of Carbohydrate Research

Taiwan: The Chemical Society Located in Taipei

Japan Society for Environmental Chemistry

The Japanese Society of Printing Science and Technology

Thailand: The Chemical Society of Thailand

Japan Society for Molecular Science

The Pharmaceutical Society of Japan

United States: American Peptide Society; Biotechnology Industry Organization (BIO); International UV Association (IUVA)

Japan Society for Safety Engineering

The Rare Earth Society of Japan

Japan Society of Colour Material

The Society for Biotechnology, Japan

Japan Society of Nutrition and Food Science

The Society of Chemical Engineers, Japan

Japan Society of Soil Science and Plant Nutrition

The Society of Fiber Science and Technology, Japan

ACKNOWLEDGMENTS



THE PACIFICHEM 2015 Organizing Committee along with the symposium organizers, gratefully acknowledge the following companies and organizations for financial and in kind contributions received in support of the Congress. We also wish to thank those who contributed but are not listed below. Additional contributors that were not available to us at press time can be found on the website at www.pacifichem.org.

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Canadian Journal of Chemistry
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| Current Polyurethane Science (#133) | Water-phase Catalysis for Energy and Chemicals Production (#182) Shell Oil Company ACS Division of Catalysis Science & Technology | Advances in the Medicinal Applications of N-Heterocyclic Carbene Metal Complexes and Azolium Cations (#255) Royal Australian Chemical Institute, Inorganic Division |
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Synthetic Modulators of Protein-Protein Interactions (#461)

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PACIFICHEM 2015

International Chemical Congress of
Pacific Basin Societies Dec. 15–20

ALOHA! Welcome to Honolulu and the 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem 2015, PAC CHEM 2015). The 2015 International Chemical Congress of Pacific Basin Societies is the seventh in the series of successful Congresses. Founded in 1984, these conferences have been held around every five years in Honolulu, Hawaii. Pacifichem's vision is to promote scientific exchange amongst chemical scientists within the pacific basin and to improve the quality of life throughout the world.

Pacifichem 2015 is sponsored jointly by the American Chemical Society (the host society), the Canadian Society for Chemistry, the Chemical Society of Japan, the New Zealand Institute of Chemistry, the Royal Australian Chemical Institute, the Korean Chemical Society and the Chinese Chemical Society. Peter J. Stang, University of Utah, is the Chair of the Congress. Steven Holdcroft, Simon Fraser University, and Eiichi Nakamura, The University of Tokyo, are the two Congress Vice Chairs, representing CSC and CSJ respectively. The theme of Pacifichem 2015 is "Chemical Networking: Building Bridges Across the Pacific."

The Congress begins on Tuesday morning, December 15 and runs through Sunday morning, December 20. There are 334 symposia focusing on 11 topical areas of chemistry: Analytical Chemistry; Inorganic Chemistry; Macromolecular Chemistry; Organic Chemistry; Physical, Theoretical & Computational Chemistry; Agrochemistry, Environmental, and Geochemistry; Biological Chemistry; Materials and Nanoscience; Chemistry of Clean Energy Conversion, Storage, and Production; Bench to Bedside: Chemistry of Healthcare; and Connecting Chemistry to Society. Information on the technical program summary listing the topical areas and the symposia can be found on page 16.

The official Congress Opening Ceremony will take place on Tuesday, December 15 at the Sheraton Waikiki Hotel in the Hawaii Ballroom from 6:00pm–7:00pm followed by the Pacifichem Lecture. The Pacifichem Lecture will feature one of New York Times bestselling authors, Sam Kean, writer for science and author of the Disappearing Spoon. Sam Kean's lecture on the Disappearing Spoon will

masterfully fuse science with the classic lore of invention, investigation, discovery, and alchemy. All registered attendees and guests are invited to attend this event. After the lecture, the Opening Reception will be held from 8:00pm–10:00pm on the Sheraton Waikiki Hotel and Royal Hawaiian Lawns. The Closing Reception will take place on Sunday, December 20 from 2:00pm–4:00pm at the Hilton Hawaiian Village in the Coral Ballroom.

More than 17,000 papers will be presented in either oral or poster formats. The Congress is utilizing the Hawaii

| CLASSIFICATION OF REGISTRANT | EARLY REG. FEES | STANDARD/ ONSITE FEES |
|--|--------------------|--------------------------|
| | JUNE 25–OCT. 15 | OCT. 16–DEC. 20 |
| Member of sponsoring or participating societies ^a | \$725 | \$825 |
| Nonmember | 850 | 950 |
| Student ^b | 250 | 250 |
| Guest | 80 | 80 |

NOTE: All fees are in U.S. dollars. **a** Member fees are available to the members of the seven cosponsoring societies and the official participating organizations. **b** Student fees are available to full-time students enrolled in an undergraduate or graduate degree program; postdoctoral fellows are not considered to be students.

GENERAL INFORMATION



Convention Center, Hilton Hawaiian Village, Hilton Waikiki Beach, Hyatt Regency Waikiki, Waikiki Beach Marriott, Royal Hawaiian and the Sheraton Waikiki for the oral technical sessions. Oral technical sessions will take place as half-day sessions in the morning [8:00am–12:00pm], afternoon [1:00pm–5:00pm] and evening [7:00pm–9:00pm]. All poster sessions will take place in the Hawaii Convention Center, Kamehameha Exhibit Halls I, II, and III.

REGISTRATION

ALL DELEGATES. All delegates must register in order to attend the Congress and technical sessions. Registration fees include attendance to the opening ceremony and reception, the Pacifichem Lecture, the closing reception, all the technical sessions, the exposition, access to meeting mail, and usage of the shuttle services. Member fees are available to members of the sponsoring societies and the official participating societies. Please see page 7 for a listing of the Sponsoring Societies and the Official Participating Societies.

ON-SITE REGISTRATION. Onsite registration is located at the Hawaii Convention Center (main lobby), the Hilton Hawaiian

Village (Coral Lounge and Lobby), the Sheraton Waikiki (Ballroom foyer, 2nd floor) and the Marriott Waikiki (Tour Lobby-Paoakalani Tower). For your convenience, program booklets and badge cases are located in all registration areas. Registration hours are: Monday, Dec. 14, 3–7pm and Tuesday, Dec. 15 through Saturday, Dec. 19, 7:30am–5:30pm; Sunday, Dec. 20, 7:30am–11:30am.

In addition to the program booklets, delegates can download the Pacifichem 2015 mobile app from the Apple Store, Google Play or Amazon. The mobile app allows attendees to browse the program by topical areas, by day, and by authors to quickly find information about the scheduling and location of sessions, author presentations, and special events. The online program at www.pacifichem.org/online will serve as the final program for Pacifichem 2015.

ATTENDEE BADGES. Attendees and guest must display their badges at all times during the conference for admittance to the technical sessions, poster sessions, expo and social events.

ON-SITE HOUSING. An on-site housing desk is located at the Hawaii Convention Center (main lobby) during the meeting to assist with last-minute housing changes or needs. On-site housing hours are: Mon-

day, Dec. 14, 3–7pm and Tuesday, Dec. 15 through Saturday, Dec. 19, 7:30am–5:30pm and Sunday, Dec. 20, 7:30am–11:30 am.

MEETING MAIL. Computer terminals with internet connections will be located at the Hilton Hawaiian Village (Coral 3), Waikiki Beach Marriott (Lobby), Sheraton Waikiki (Ballroom Foyer, 2nd floor), and the Hawaii Convention Center (Third floor).

CONGRESS INFORMATION CENTERS.

Information booths will be located in the registration areas of the Hawaii Convention Center, Hilton Hawaiian Village, and the Sheraton Waikiki. The hours of operation are Monday, Dec. 14, 2pm–7pm; Tuesday, Dec. 15, 7:30am–7:30pm; Wednesday, Dec. 16, through Saturday, Dec. 19, 7am–5pm; Sunday, Dec. 20, 7am–11am.

LOST AND FOUND. Items lost or found in meeting rooms should be turned in to Pacifichem Operation Offices at the official hotels or the Hawaii Convention Center. Attendees can claim lost items from the operation offices. Items not claimed from the operation offices by the end of the conference will be turned in to security at the Official Hotel or Hawaii Convention Center.

DAYCARE SERVICES: Most of the official hotels on the Pacifichem hotel list have babysitting services or can refer guests to a babysitting service. For more information or to make arrangements, contact the Guest Services Desk of the hotel. The co-sponsoring societies can't be held liable or responsible for care given by these child care services.

FACILITIES FOR PEOPLE WITH

DISABILITIES. We are committed to making the Congress accessible to all people. We realize some people may have special requirements, such as interpreters for the hearing impaired and shuttle vehicles with lifts. Facilities utilized for the meeting are readily accessible. If you have special needs during the meeting, contact the nearest Congress Operations Office for assistance.

SHUTTLE SERVICES. The Pacifichem shuttle bus will operate between the Hawaii Convention Center and the official Pacifichem hotels every 15 minutes during rush hours and 30 minutes during non-rush hours beginning December 15 (7am–5:30pm then 5:30pm–10:30pm to the Opening Cer-

WORKSHOPS

WEDNESDAY, DEC 16, 2015 • 7:00PM–9:00PM

COMMUNICATING YOUR RESEARCH CLEARLY AND EFFECTIVELY

Hawaii Convention Center, Room 304A

The advancement of science depends on sharing research findings. Most scholarly journals are published in English, and it's important to be able to clearly communicate in these journals. In the past year, we edited over 10,000 physical science manuscripts for researchers throughout the world who don't speak English as a first language. In this workshop, we will discuss how to communicate research clearly and effectively in a scholarly manuscript. We will also cover mistakes commonly made when writing in English. Finally, we will conclude with a discussion on how to convey findings in a brief and effective way for a general audience.

WEDNESDAY, DEC 16, 2015 • 7:00PM–9:00PM

DOING BUSINESS WITH THE DEFENSE THREAT REDUCTION AGENCY (DTRA)

Hilton Hawaiian Village, Kalia Tower, Lehua Suite

This workshop will focus on the Defense Threat Reduction Agency's (DTRA) Research and Development Dire.

THURSDAY, DEC 17, 2015 • 7:00PM–9:00PM

APPLYING TO GRADUATE SCHOOL IN THE US: WORKSHOP WITH FACULTY

Hawaii Convention Center, Room 303A

Many college students outside the U.S. are interested in attending graduate school in chemistry and biochemistry in the United States. We will discuss common questions about the admissions process, expectations, and funding for graduate students in the U.S. Interested students are welcome to participate in a Q&A session.

THURSDAY, DEC 17, 2015 • 7:00PM–9:00PM

Leadership and Following

Hilton Hawaiian Village, Kalia Tower, Kahili Room

Leadership in Science will reflect on some necessities of leadership in academia and industry: How to communicate with people? How to delegate and how to listen? The workshop will be led by Alexander Schiller, chemist and Junior Professor at University Jena, Germany.

THURSDAY, DEC 17, 2015 • 7:00PM–9:00PM

How to Review a Manuscript

Hilton Hawaiian Village, Nautilus I Room

In this hands-on Reviewer Workshop, young researchers will be trained in the art of peer review. The Participants will be sent a manuscript in advance which they have to review. During the Workshop Angela Wilson (Editor of Computational and Theoretical Chemistry and Director of the NSF Division of Chemistry) will go through the article step by step together with the young scientists. Those interested should contact Rob van Daalen at G.Daalen@elsevier.com or Evalyne Wanjiru at e.wanjiru@elsevier.com

emony only). Shuttles will continue running from 7am–10pm, December 16–19; and from 7am–noon, December 20; and 1pm–4pm to the Closing Ceremony. Additional information on the shuttle schedules can be found in the lobby areas of the official hotels and the Hawaii Convention Center.

ADA requests for shuttle reservations should be made at least 7 days in advance by contacting Naomi Aquino at Naomi-Laguino@robertshawaii.com. cc: group-sales@robertshawaii.com or by calling 888-

472-4729 or 808-539-9481. Call the dispatch hot line for same day reservations at 808-831-1555 (may incur a 30 minute wait time).

SPEAKER INFORMATION. Speaker Check-In Procedures: It is strongly recommended that all speakers visit the Speaker Ready Room (In the building they will be presenting) 24 hours in advance of their presentation. Each hotel and convention center will have a speaker ready room where speakers can view their presentation(s) in order to avoid compat-

ibility issues with the computer supplied in the meeting room. Technicians will also be available to assist speakers with uploading their presentations to the computer that will be in the session room.

All electronic files must be submitted in the Speaker Ready room in either PowerPoint or PDF format. Note: Users of PowerPoint 2007 or later should save their file in the native pptx format for greatest compatibility.

Presenters should bring their files on a PC Formatted USB drive. Note: If you have a QuickTime videos as a part of your presentation, please make sure to submit the presentation to the Speaker Ready Room at least 24 hours in advance due to additional time that may be required to re-encode the videos.

Internet connectivity is not available in oral session rooms unless it has been ordered and paid for by the session organizers in advance.

The standard audiovisual equipment provided for technical sessions will consist of a computer (With a wired mouse), a computer projector, switcher, screen, lighted podium, podium microphone, lapel microphone and a laser pointer. The laptop computer will have the following configuration:

- Processor: a minimum i7 2.2 GHz
- 8 Gig RAM
- 1024 x 768 at 24 bit color depth
- Microsoft Office 2010
- Windows Media Player (Latest Version)
- Quick Time (Latest Version)
- Flash Player (Latest Version)
- Adobe Acrobat Reader (Latest Version)

Please refer to the following website for tips on formatting your presentation: <http://www.projectionnet.com/styleguide/presentationstyleguide.aspx>. Technical questions should be sent to the ACS audio-visual provider: acs@projection.com

SPEAKER READY ROOM HOURS:

Monday, December 14

3:00pm–7:00pm

Tuesday, December 15

7:00am–8:00pm

Wednesday, December 16

7:00am–8:00pm

Thursday, December 17

7:00am–8:00pm

Friday, December 18

7:00am–8:00pm

Saturday, December 19

7:00am–8:00pm

Sunday, December 20

7:30am–11:30am

GENERAL INFORMATION

TRANSPORTATION. Delegates arriving at the Honolulu International Airport will arrive at the main terminal located on the second level. Proceed to the escalator or elevator down to the ground floor to access baggage claim areas and ground transportation. Visitor information booths are located in gate and baggage claim areas to assist arriving passengers.

GROUND TRANSPORTATION. Taxi service is available at the Honolulu International Airport on the center median fronting the terminal baggage claim areas. See the taxi dispatchers in yellow shirts with black lettering (TAXI DISPATCHER) for service. The fare from the airport to Waikiki during non-rush hour periods is approximately \$40.00–\$45.00, plus a baggage charge of 50 cents per bag. Fare is by meter only.

CITY BUS. The City & County of Honolulu provides an island-wide bus transportation system that serves Honolulu International Airport. Children up to 5 years of age ride free. The fare for children and students (6–17) is \$1.25; Adults-\$2.50; senior citizens (with reduced fare card or valid US Medicare card is \$1.00; and a visitor's pass (four consecutive days pass with unlimited use)–\$25. For route information visit www.thebus.org or call customer service at (808) 848-4500 or call (808) 848-5555.

TOURS. Pacifichem attendees will receive a 20% discounted rate on tours booked through Roberts Hawaii of Oahu, Maui, Kauai and Hawaii Island. Confirmations will be sent directly from Roberts Hawaii listing the location of departure and the pickup time. Tours can be purchased online at www.robertshawaiexpress.com or by calling (800) 831-5541 (US/Canada) between 7am–9pm HST using promo code: PACHEM15.

AIRPORT SHUTTLE. Roberts Hawaii Express Shuttle provides affordable transportation from the Honolulu International Airport to hotels along Oahu for a discounted rate of \$12.80 (one way) and \$24.00 (round trip). Roberts Hawaii Express airport representatives will meet and greet attendees upon arrival and assist with their luggage at the baggage claim area. Transportation fee includes 2 pieces of luggage and a personal carry on complimentary. Golf bags may be considered 1 piece of luggage. Additional luggage over 2 per person will cost an additional fee. Due to limited availability, Roberts Hawaii requires that ADA vehicle reservations be made a minimum of 48 hours prior to the date and time of service. Reservations for transportation can be made by calling the Reservations Office at 1(800) 831-5541 (US/Canada) between 7am–9pm HST or via online at www.robertshawai.com/pachem2015 using promo code: PACHEM15. Advanced reservations required. A 10% service fee will be charged for credit card booking cancellations. There will be no charge for cancellations made by 12 noon, the day prior to the date of the scheduled service. Round trip scheduled service is defined as the first date of the round trip booking. Thereafter, a full charge will apply. No refund will be given for cancellation notices within 24 hours of service date/time and no shows are subject to the full charge. Should you have questions, email Roberts Hawaii at airport.shuttle@robertshawai.com or call 1 (800) 831-5541 (US/Canada) or (808) 441-7800.

son will cost an additional fee. Due to limited availability, Roberts Hawaii requires that ADA vehicle reservations be made a minimum of 48 hours prior to the date and time of service. Reservations for transportation can be made by calling the Reservations Office at 1(800) 831-5541 (US/Canada) between 7am–9pm HST or via online at www.robertshawai.com/pachem2015 using promo code: PACHEM15. Advanced reservations required. A 10% service fee will be charged for credit card booking cancellations. There will be no charge for cancellations made by 12 noon, the day prior to the date of the scheduled service. Round trip scheduled service is defined as the first date of the round trip booking. Thereafter, a full charge will apply. No refund will be given for cancellation notices within 24 hours of service date/time and no shows are subject to the full charge. Should you have questions, email Roberts Hawaii at airport.shuttle@robertshawai.com or call 1 (800) 831-5541 (US/Canada) or (808) 441-7800.

CAR RENTALS. Hertz, Enterprise, and Dollar Rent A Car are offering discounted rates for Pacifichem 2015. Contact Hertz at (800) 654-2240 and refer to code: CV#022Q7358; for Enterprise call (800) 593-0505 using code: 32H7476; and for Dollar Rent A Car call (800) 800-3665 using code: CM0679.

SPECIAL EVENTS

CONGRESS OPENING CEREMONY. Tuesday, Dec. 15, 6:00pm–7:00pm, Sheraton Waikiki Hotel, Hawaii Ballroom. The ceremony will open with welcoming remarks from the chair of the Congress.

PACIFICHEM LECTURE. Tuesday, Dec. 15, 7:00pm–8:00pm, Sheraton Waikiki Hotel, Hawaii Ballroom. Sam Kean, one of New York Times bestselling authors will give the Pacifichem 2015 lecture on “The Disappearing Spoon”. The lecture will detail how the periodic table masterfully fuses science with the classic lore of invention, investigation, and discovery.

CONGRESS OPENING RECEPTION. Tuesday, Dec. 15, 8:00pm–10:00pm will be held on the Sheraton Waikiki Hotel and Royal Hawaiian Lawns. All delegates and guests are welcome.

EXPOSITION. Tuesday, Dec. 15 (2pm–5pm), Wednesday, Dec. 16 (11am–5pm), and Thursday, Dec. 17 (11am–5:30pm) in the Coral Lounge & Ballroom at the Hilton Hawaiian Village.

STUDENT POSTER COMPETITION.

Tuesday, Dec. 15, noon–2pm, Hawaii Convention Center, Kamehameha Exhibit Halls I, II & III. Approximately 350 student finalists selected from over 7,500 Pacifichem poster submissions will participate in the competition. Open to student poster competition finalist only.

CLOSING RECEPTION. Sunday, Dec. 20, 2:00pm–4:00pm, Hilton Hawaiian Village, Coral Ballroom, Mid Pacifichem Conference Center. The Orchestra Chemica Japan will provide Chamber music. All delegates and guests are welcome.

POSTER SESSIONS. Poster presenters must register for the meeting. All poster sessions will be located at the Hawaii Convention Center in Kamehameha Halls I, II & III. The poster boards provided will be 4 feet high and 8 feet wide. Presenters are responsible for mounting their material on the poster boards prior to the opening of the poster sessions. Boards will be numbered with designated poster numbers and pushpins will be provided to mount posters. Boards are available for poster setup one hour prior to the start time of the session. Posters should be removed within a half hour after the session ends. Pacifichem cannot assume responsibility for materials beyond these time limits. Authors must be present by their posters during the time of their poster session.



MEDICAL BREAKTHROUGHS MAY COME OUT OF THE LAB.
BUT THEY BEGIN IN THE HEART.

For more than 150 years, a very special passion has driven the people of Merck. Our goal is to develop medicines, vaccines, and animal health innovations that will improve the lives of millions. Still, we know there is much more to be done. And we're doing it, with a long-standing commitment to research and development. We're just as committed to expanding access to healthcare and working with others who share our passion to create a healthier world. Together, we'll meet that challenge. With all our heart.

For more information about getting Merck medicines and vaccines for free, visit merckhelps.com or call 800-727-5400.



TECHNICAL PROGRAM SUMMARY

Topic Areas

I. The Core Areas of Chemistry

- 01. ANYL - Analytical
- 02. INOR - Inorganic
- 03. MACR - Macromolecular
- 04. ORGN - Organic
- 05. PHYS - Physical, Theoretical & Computational

II. Multi- & Cross-Disciplinary Areas of Chemistry

- 06. ENVR - Agrochemistry, Environmental & Geochemistry
- 07. BIOL - Biological
- 08. MTLs - Materials & Nanoscience

III. Chemistry Solutions to Global Challenges

- 09. ENRG - Chemistry of Clean Energy Conversion, Storage & Production
- 10. HLTH - Bench to Bedside: Chemistry of Health Care
- 11. SCTY - Connecting Chemistry to Society

| 01. Analytical | A | N | Y | L | | | |
|--|---|----|----|----|----|----|--|
| Marriott Waikiki Beach | T | W | T | F | S | S | |
| New Tools & Methodologies for the Characterization of Biomolecular Interactions (#15) | D | D | P | TA | | | |
| Development & Applications of Techniques for Electrochemical Analysis (#24) | | | D | D | TA | | |
| Current Issues in Teaching Analytical Chemistry (#38) | | D | TA | | | | |
| Frontiers in Flow Injection Analysis & Related Techniques (#45) | D | D | TA | | | | |
| Supercritical Fluid Chromatography (SFC) for Analysis & Purification (#53) | | D | TE | | | | |
| Advances in Analytical Ion Mobility Separations (#61) | D | D | TA | | | | |
| On-site & In Vivo Instrumentation & Applications (#88) | | D | TE | | | | |
| Direct & Mediated Bioelectrocatalysis for Biosensors & Energy Conversion Applications (#89) | | | | D | A | TE | |
| Comprehensive Multidimensional Separations (#90) | | | | P | A | | |
| Immunoanalysis: Applications & Trends for Environmental Monitoring & Human Health (#94) | D | D | TA | | | | |
| Novel Analytical Probes for In Vivo Optical Functional Imaging (#115) | | | | P | D | A | |
| Micro- & Nanofabricated Analytical Devices for Chemical, Biochemical & Biomedical Platforms (#129) | D | DE | AE | TA | | | |
| Marine & Freshwater Toxins: Detection, Structure & Pharmacology (#138) | | | | D | A | TE | |
| Innovation in Chemical Sensing & Separation Systems toward Advanced Chemical Analysis (#159) | D | TA | | | | | |
| Fundamentals & Applications of Atomic Spectrometry (#160) | D | D | | | | | |
| Optical Waveguide Techniques for the Analyses of Materials & Interfaces (#164) | | | D | A | | | |

A = Oral AM P = Oral PM E = Oral Eve D = Oral AM/PM
 TA = Poster AM TE = Poster Eve

All posters sessions are located at the Hawaii Convention Center.

01. Analytical (continued)

A N Y L

| Marriott Waikiki Beach | T | W | T | F | S | S |
|--|---------|---------|---------|---------|---|---|
| Paper-Based Analytical Devices for Point-of-Need Measurements (#213) | | | | P TE | A | |
| Symposium on Petroleomics: Molecular-Level Understanding of Petroleum for Environmental Science & Petroleum Engineering (#247) | D | TA | | | | |
| Laser Ionization Mass Spectrometry (#274) | | | D | | | |
| Ultrasensitive Assays for Proteins & Protein Modifications (#287) | | DE | E TA | | | |
| Advanced Analytical Applications & Technical Developments of Soft X-Ray Spectroscopy (#303) | | | P TE | D | | |
| Advances in FTIR Microspectroscopy: 3-D Tomography to Nanoscale Imaging (#315) | | D TE | | | | |
| Magnetoanalytical Science: Separation, Characterization & Imaging (#320) | D TE | A | | | | |
| Harmonized Strategy of New UHPLC Implementation in Pharmaceutical R&D & CRO/CMO QC Laboratories (#353) | | | A | | | |
| Vibrational Spectroscopy: New Developments & Applications in Biological & Medical Sciences (#375) | | | D TE | | | |
| Analytical Laser-Induced Breakdown Spectroscopy (LIBS) for Hazards Analysis, Forensics & Health (#379) | | | | P TE | A | |
| Bacterial Identification by Mass Spectrometry (#389) | | | | A TE | | |
| Advances in Analytical Techniques for Effective Food Allergen Management (#394) | | | | P TE | A | |
| Advances in Terahertz Spectroscopy & Imaging (#413) | | | D TE | | | |
| (Bio-)Chemical / Electrochemical Sensors & Sensing Materials (#417) | P TA | D | | | | |
| Plasmonic Materials for Chemical Analysis (#450) | P TA | D | | | | |
| Organized Surfactant Assemblies in Chemical Analysis & Separation Science: Fifty Years Later (#457) | | | | D TE | A | |
| Analytical General Posters | TA | | | | | |

02. Inorganic (continued)

I N O R

| Hilton Hawaiian Village | T | W | T | F | S | S |
|---|---|---------|----|---------|---------|------|
| Organo-Main Group Avenues toward Advanced Materials (#16) | D | D | TA | | | |
| Fundamentals & Applications of Solvent Extraction in the Recovery of Strategic Metals (#17) | D | D | | | | |
| Experimental & Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42) | | | | DE | D TE | A |
| Metal-Organic Frameworks: Synthesis, Properties & Applications (#50) | | | | E | D TE | A |
| From Pnictides to Perovskites: Impact of Local Structure in Solid-State Chemistry (#62) | | | | PE | D TE | A |
| Lewis Acid-Base Pair Chemistry in Molecular Transformations, Catalysis & Energy Storage (#65) | D | D TE | | | | |
| Functional Nanomaterials Based on Coordination Chemistry (#73) | | | | D TE | A | |
| Molecular Catalysis of Water-Splitting Reactions (#76) | D | D | TA | | | |
| Accessing the Full Potential of Redox-Active Ligands: Reactivity & Applications (#87) | | | | | D TE | A |
| Recent Discoveries in the Chemistry of Bismuth & Related Elements: The Green Alternative (#93) | | | | | D | A |
| Coordination & Supramolecular Chemistry for Aqueous Metal Ion Separations (#97) | | | | D TE | D | |
| Frontiers of Molecular Magnetism (#109) | | | | D TE | D | |
| Frontiers of Organo-f-element Chemistry (#125) | D | D | TA | | | |
| Electron Transfer & Electrochemistry of Inorganic & Organometallic Materials (#126) | | | | P TA | D | |
| Chemistry & Application of Boron Clusters (#152) | | | | | TE | DE A |
| Current Trends & Interconnectivities Among Fundamental & Applied Inorganic Fluorine Chemistry (#156) | | | | P TE | D | A |
| Noncovalent Interactions in Coordination Systems (#161) | D | D | TA | | | |
| Activation & Transformation of Small Molecules Mediated by Early-Transition-Metal Complexes (#170) | | | | DE | D TE | |
| Innovative Approaches in Bond-Cleavage & Bond-Forming Reactions at Late-Transition-Metal Centres (#186) | D | D | TA | | | |

PROGRAM SUMMARY

02. Inorganic (continued)

I N O R

| Hilton Hawaiian Village | T | W | T | F | S | S |
|---|---------|---------|----|---------|---|---|
| Transition-Metal Complexes of N-Heterocyclic & Mesoionic Carbenes: Structure, Materials & Catalytic Applications (#195) | | D TE | A | | | |
| Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus & Synthesis (#226) | | | | D TE | A | |
| The Expanding Periodic Table: New Discoveries & Chemistry of the Heaviest Elements (#234) | | | | D TE | A | |
| Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239) | | P TE | D | | | |
| Nuclear Probes in Nanoscale Characterization (#254) | DE | TA | | | | |
| Advances in the Medicinal Applications of N-Heterocyclic Carbene Metal Complexes & Azolium Cations (#255) | | | | D TE | | |
| Inorganic Complexes for Solar Energy Harvesting (#256) | | P | D | TA | | |
| Metal-Containing π -Conjugated Systems: Syntheses, Properties, Applications (#269) | D | TA | | | | |
| Metal Mediated Polymerization (#292) | | D | D | TA | | |
| s Block Metal Chemistry (#304) | | | | D TE | A | |
| Novel Heme Proteins & Model Systems (#305) | | D TE | A | | | |
| Metal Coordination Sphere Design for Challenging Bond Transformations (#318) | | DE | D | P TA | | |
| Dioxygen Activation Chemistry of Metalloenzymes & Models (#339) | D TE | A | | | | |
| New Frontiers in Bioinorganic Chemistry (#356) | D | D | TA | | | |
| Isotope Production—Providing Important Materials for Research & Applications (#363) | D TE | A | | | | |
| The Biocoordination Chemistry of Nitric Oxide & Its Derivatives: Mechanisms of NO _x Generation, Signaling & Reduction in Biological Systems (#371) | | | TE | DE | A | |
| Dynamic Aspects of Solid Materials: From Equilibrium to Nonequilibrium Systems (#376) | D | TA | | | | |
| Activation of Small Molecules by Electropositive Metals Related to Chemical Energy Conversion (#380) | | | | D TE | A | |

02. Inorganic (continued)

I N O R

| Hilton Hawaiian Village | T | W | T | F | S | S |
|--|---|---|---|---------|---------|---|
| New Directions for Sensing Metals in Biology (#424) | | | | | D TE | A |
| Telomeres & Other G-quadruplex Structures as Targets for Metallodrugs (#459) | | | | D TA | | |
| Inorganic General Posters | | | | | TA | |

03. Macromolecular

M A C R

| Hawaii Convention Center | T | W | T | F | S | S |
|--|--------------|----|---------|----------|---------|---|
| NMR Spectroscopy of Polymers & Biobased Materials (#12) | E TA | | DE | DE | A | |
| Synthetic Biopolymers (#37) | D A TE | | | | | |
| New Perspectives of Synthetic & Biological Soft Matter (#57) | | | D TE | DE | | |
| Dynamic, Reversible & Self-Healing Materials (#64) | | | | | P TE | A |
| Polymer Gels as Advanced Soft Materials (#83) | D | DE | TA | | | |
| Radical Polymerization Kinetics & Process Modeling (#92) | | | | | D | A |
| New Frontiers in Polymer Crystallization (#96) | | | | PE TA | D | A |
| Simulation of Polymers (#110) | D TA | | | | | |
| Controlled Macromolecular & Supramolecular Architectures for Sustainability (#112) | D D | TA | | | | |
| Current Polyurethane Science (#133) | | | | | D TE | A |
| Monomer Sequence Control: Using Nature's Strategy to Create 21st-Century Polymers (#158) | | | DE | D TE | | |
| Characterization of Polymers & Polymer Assemblies in Solution (#172) | D TE | A | | | | |
| Polymer Interfaces: Design, Structure, Physical Properties & Applications (#194) | P TE | D | A | | | |
| Macromolecular Self-Assembly for Smart Biomaterials (#196) | | | | P TE | D | A |
| Functional Materials Based on Organic-Inorganic Hybrid Polymers (#221) | D D | TA | | | | |

A = Oral AM P = Oral PM E = Oral Eve D = Oral AM/PM
 TA = Poster AM TE = Poster Eve

All posters sessions are located at the Hawaii Convention Center.

03. Macromolecular (continued)

M A C R

| Hawaii Convention Center | T | W | T | F | S | S |
|---|---------|---|---------|---------|----|---|
| Cyclic & Topological Polymers (#248) | | | | P TE | D | A |
| Advanced Membrane Separations (#262) | | | | TE | DE | A |
| Polymers from Renewable Sources & Sustainable Polymer Synthesis (#281) | D TE | D | | | | |
| Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic & Inorganic Components (#294) | | | | P TE | DE | A |
| Sustainable Conversion of Lignin to Value-Added Products & Green Chemicals (#319) | D TE | D | | | | |
| Polymers for Energy & Optoelectronic Devices (#361) | D TE | D | | | | |
| Polymer Materials Performance, Degradation & Optimization (#369) | | | D TE | A | | |
| New Perspectives of Bioplastics for Environmental Benign Materials (#396) | | | D TE | A | | |
| Advances in Precision Polymer Synthesis Using Reversible-Deactivation Radical Polymerization (#401) | | | D TE | A | | |
| Aggregation Induced Emission: Materials & Applications (#444) | | | DE | D TA | P | A |
| Macromolecular General Posters | TA | | | | | |

04. Organic (continued)

O R G N

| Hilton Hawaiian Village | T | W | T | F | S | S |
|---|---------|---------|---------|---------|---------|----|
| Molecular Containers (#99) | | | | D TE | A | |
| Organoboron Chemistry: Applications in Organic Synthesis, Biology & Materials (#100) | | | P TE | D | D | |
| Electrochemical Reactions & Mechanisms in Organic Chemistry (#104) | | | | D TE | | |
| Recent Trends in Organocatalysis (#122) | | | | DE | DE | TA |
| Organic Reactions in Aqueous Media (#131) | | | | | D | |
| Practical Application of Basic Research on Molecular Recognition (#136) | | | D TE | | | |
| New Green Techniques for Medicinal Chemistry (#148) | | | | | D TE | A |
| Applications of C–H Functionalization (#169) | | | | DE | D TE | A |
| Strategies & Tactics for Complex Molecule Synthesis (#174) | | | | DE | D TE | A |
| Homogeneous Gold Catalysis: Methods, Theories & Applications (#192) | D TE | A | A | | | |
| Molecular Function of Natural Products: Advances toward Chemical Biology (#237) | D DE | DE | TA | | | |
| The Science & Strategy of Pharmaceutical Process Chemistry: Adapting to Global Regulatory Development Guidance on Process Impurities (#242) | | | D TE | | | |
| Molecular Self-Assembly & Functional Organic Nanostructures (#263) | | | D TE | | | |
| Cooperative Cocatalysis with Two Different Metals (#270) | | | | | D TE | A |
| Molecular Probes & Fluorophores for Biological Imaging (#280) | | | D TE | A | | |
| Frontiers of Chirality in Organic Chemistry (#286) | D DE | DE | TA | | | |
| Supramolecular Chemistry at the Interface of Materials, Biology & Medicine (#300) | D TE | A | | | | |
| Chemical Glycosylation: Methods & Mechanisms (#306) | | | | P TE | D | A |
| Fluorinations & Fluoroalkylations (#310) | | P TE | D | | | |
| Nanomaterials as Catalysts for Green Chemistry (#313) | D A | A TE | | | | |
| Mechanochemistry & Solvent-Free Synthesis (#322) | D TA | | | | | |

04. Organic

O R G N

| Hilton Hawaiian Village | T | W | T | F | S | S |
|---|---------|---------|---------|---------|---|---|
| Reactive Intermediates & Unusual Molecules (#7) | | DE | A TE | | | |
| Designed π -Electronic Systems: Synthesis, Properties, Theory & Function (#25) | | | P TE | D | D | |
| Prospects for Flow Chemistry (#29) | D TE | D | | | | |
| Anion Receptors (#31) | | | | P TE | D | A |
| Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes & Related Materials (#41) | | P TE | DE | A | | |
| Natural-Product-Based Drug Discovery (#66) | | | D TE | D | D | |
| Molecular & Supramolecular Photochemistry (#71) | D DE | DE | TA | | | |
| Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74) | D TE | D | | | | |

PROGRAM SUMMARY

04. Organic (continued)

O R G N

| Hilton Hawaiian Village | T | W | T | F | S | S |
|--|--------------|----|----------|---------|---|---|
| Carbenes & Carbeneoids in Organic Synthesis (#362) | D | TA | | | | |
| Organic Solid-State Chemistry: Structure, Property & Reactivity (#398) | P TE | D | A | | | |
| Cognizance of Endangered Elements for Organic Synthesis (#415) | D A TE | | | | | |
| New Horizon of Process Chemistry by Scalable Reactions & Technologies (#426) | | | P TE | D | | |
| New Organosulfur Chemistry (#436) | | | DE TE | A | | |
| Photoredox Catalysis in Organic Synthesis (#440) | D TE | | | | | |
| Asymmetric Supramolecular Catalysis (#451) | | | | D TE | | |
| Catalytic Multicomponent, Tandem & Cascade Reactions (#455) | D TE | | | | | |
| Synthetic Modulators of Protein-Protein Interactions (#461) | | | P TE | D | A | |
| Organic General Posters | TA | | | | | |

05. Physical, Theoretical & Computational (continued)

P H Y S

| Hawaii Convention Center | T | W | T | F | S | S |
|---|----|---------|---------|----------|----|---|
| Deciphering Molecular Complexity from Single Molecules to Cellular Networks (#121) | D | D | | | | |
| Recent Advances in Dynamics of Confined Liquids (#123) | | | | P TE | DE | A |
| Computational Modeling of d- & f-Block Chemistry: Challenges & Opportunities (#130) | D | D TE | | | | |
| Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134) | D | D TE | | | | |
| Recent Progress in Molecular Theory for Excited-State Electronic Structure & Dynamics (#142) | D | DE | E TA | | | |
| Self-Organization in Chemistry (#165) | | | D TE | D | | |
| Frontiers of Metal Clusters & Nanostructures: From Fundamental Properties to Functionalities (#168) | D | D TE | | | | |
| Challenges in Plasmonic Photochemistry (#176) | | | | P TE | D | A |
| Theory of Main Group Chemistry Beyond First Row (#183) | D | TA | | | | |
| Challenges & Opportunities for Exascale Computational Chemistry (#184) | | | | P | D | A |
| Latest Development of Advanced Vibrational Spectroscopy (#187) | D | D TE | | | | |
| Recent Progress in Matrix-Isolated Species (#199) | | | | DE TE | A | |
| Metal Ions & Protein Functions: Theoretical Models & Applications (#202) | | | | DE TE | D | |
| Quantum Fluid Clusters (#203) | | | | | DE | A |
| Single-Molecule Fluorescence Imaging (#208) | DE | D TE | | | | |
| Molecular Perspectives on Interfacial Electrochemistry & Electrocatalysis (#218) | | | | PE TA | DE | A |
| Fundamental Science of Photon- & Electron-Induced Surface Processes (#228) | PE | DE | A | | | |
| Interplay between Theory & Experiment in Catalytic Research (#277) | DE | D | TA | | | |
| Quantum Coherence in Energy Transfer (#297) | | | | D D | A | |

A = Oral AM P = Oral PM E = Oral Eve D = Oral AM/PM
 TA = Poster AM TE = Poster Eve

All posters sessions are located at the Hawaii Convention Center.

05. Physical, Theoretical & Computational (continued)

| | P | H | Y | S | | |
|--|---------|---------|---------|---------|---|---|
| Hawaii Convention Center | T | W | T | F | S | S |
| Dynamical Intermolecular Interactions for Biological Functions (#307) | | | P | DE | A | |
| Science with Beams of Radioactive Isotopes (#340) | | | D | A | | |
| Photocatalysis & Charge Transfer at Interfaces & Nanomaterials (#344) | TE | DE | AE | | | |
| Dissociation of Biomolecules in the Gas Phase for Structural Characterization (#352) | | | | D | A | |
| Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology & Materials (#370) | D TE | D | | | | |
| Practical Strategies for Modeling Noncovalent Interactions (#372) | | D TE | A | | | |
| Advances in Quantum Dynamics from Spectroscopy to Reactions (#384) | | | D TE | A | | |
| Interfacial Phenomena for Bubbles, Droplets, Films & Soft Matter (#403) | | D | D TE | A | | |
| Frontier Chemical Applications Using Accelerator-Based Photon Sources (#414) | D | TA | | | | |
| Reactive Intermediates in Combustion & Atmospheric Chemistry (#419) | | E | DE | D TE | A | |
| Frontiers of Photon Upconversion Based on Triplet-Triplet Annihilation (#420) | D | TA | | | | |
| Computational Modeling of Magnetic Materials & Magnetic Properties (#423) | D | | | | | |
| Frontiers of Plasmon-Enhanced Spectroscopy (#428) | D | DE | TA | | | |
| Recent Experimental & Theoretical Advances in Studies of Liquid Interfaces (#437) | | | P | D TE | A | |
| Developments in Spectroscopic Investigation of Intermolecular Interactions & Dynamics of Molecular Clusters (#438) | D | DE | E TA | | | |
| Interplay between Chemistry & Dynamics in Biomolecular Machines (#441) | | DE | TA | | | |
| Structure & Spectroscopy of Linear Polyenes: Finite & Infinite (#456) | | D TE | A | | | |
| Physical, Theoretical & Computational General Posters | | | TA | | | |

06. Agrochemistry, Environmental & Geochemistry (continued)

| EN V R | T | W | T | F | S | S |
|---|---------|---------|---------|---------|---|---|
| Hilton Waikiki Beach | T | W | T | F | S | S |
| Ferrites & Ferrates: Chemistry & Applications in Sustainable Energy & Environmental Remediation (#13) | | D TE | D | | | |
| Chemicals of Emerging Environmental Concern: A Global Perspective (#19) | | | DE | D TE | | |
| Pectin Chemistry & Technology (#20) | | | | P | D | A |
| Human Exposure to Environmental Contaminants (#26) | | | | D TE | A | |
| Recycling of Polymeric Materials: Challenges & Perspectives (#36) | | | | D TE | A | |
| Analysis of Flavors in Specialty Asian Foods (#58) | | | D TE | | | |
| Advanced Products from Lignin & Micro- or Nanofibrillated Cellulose (#70) | | P | D | TA | | |
| Application of Mass Spectrometry to Agrochemical Challenges (#72) | D | TA | | | | |
| Nanointerfaces & Their Role in Environmental Systems & Processes (#86) | D | D TE | | | | |
| Sustainable Chemistry: Beyond the Bench (#103) | D | A TE | | | | |
| Chemical Ecology Applied to Sustainable Agriculture (#105) | | | P TE | D | | |
| Chemistry & Biology of Auxin, Strigolactone & Their Interactions (#107) | D TE | | | | | |
| UV Photochemistry for Water: Implications for Safe Water Disinfection & Oxidation Treatment Applications (#204) | D | DE | TA | | | |
| Enzymes Essential to Biosphere Health: Bioremediation & Biogeochemical Cycling (#219) | | | | P TA | A | |
| Fate & Risks of Nanoparticles in Aquatic & Terrestrial Environments (#220) | | | P TE | A | | |
| Complex Mineral Growth & Dissolution Reactions: Collaborative Experimental & Computational Perspectives (#225) | | D TE | | | | |
| Proteomics & Metabolomics in Agricultural, Environmental & Public Health Sciences (#264) | | | D TE | | | |
| Genomics & Metabolomics for Phytochemical Research (#267) | D | TA | | | | |
| Opportunities & Advancements in Rice Research & Aquaculture Research (#282) | | A TE | | | | |

PROGRAM SUMMARY

06. Agrochemistry, Environmental & Geochemistry (continued)

E N V R

Hilton Waikiki Beach

| | T | W | T | F | S | S |
|--|---------|---------|---------|---------|---|---|
| Analytical Development Relevant to Environmental Exposure & Effects (#288) | | | | D TE | | |
| Advances in Functional Foods & Flavor Chemistry Research (#329) | | | DE | D TE | | |
| Environment & Gene Interaction (#336) | | D | | | | |
| Phytochemicals for Crop Protection: Discovery to Molecular Target (#358) | D | TA | | | | |
| Fukushima & Radiological Contaminated Environments Worldwide: The Important Role of Environmental Chemistry & Radiochemistry in Remediation & Restoration (#374) | | D | TE | | | |
| Radioactive Contaminants & Waste Management in the Environment (#390) | | | D TE | | | |
| Sources, Fates & Risks from Consumer Product Ingredients in the Environment (#391) | D | TA | | | | |
| Food Processing: Chemistry, Quality, Safety, Sustainability & Value-Added By-Products (#400) | D TE | D | | | | |
| Status & Trends of Persistent Organic Chemicals in the Environment (#402) | | D TE | | | | |
| Chemistry of Integrated Water Treatment Systems for Halogenated Organics & Long-Lived Radionuclides (#454) | | | | D TE | | |
| Agrochemistry, Environmental & Geochemistry General Posters | | TA | | | | |

07. Biological

B I O L

Sheraton Waikiki (*) & Royal Hawaiian (**)

| | T | W | T | F | S | S |
|---|---|---------|----------|----------|--------|---|
| Advances in Peptide & Protein Chemistry (#6) (*) | | | P TE | D DE | A | |
| Functional Nucleic Acids: Chemistry, Biology & Materials Applications (#10) (*) | | | | AE TE | D A | |
| New Platforms for Natural Products Discovery (#18) (**) | E | D TE | D | | | |
| Biosynthesis of Natural Products (#27) (*) | | | PE TA | DE | A | |
| Homeostasis of Transition-Metal Ions in Biological Systems (#47) (*) | | | | D TE | A | |

07. Biological (continued)

B I O L

Sheraton Waikiki (*) & Royal Hawaiian (**)

| | T | W | T | F | S | S |
|--|---------|---------|----|---------|---------|---|
| Characterization & Applications of Food Enzymes (#59) (*) | | | | D TE | | |
| Heat-Shock Proteins: The Next Target in the Disease Frontier (#91) (*) | | | | | D TE | |
| Low-Energy Photoexcited States in Photosynthesis (#117) (*) | D | D | | | | |
| Advances in Biological Solid-State NMR (#120) (**) | D | DE | TA | | | |
| Life at Small Copy Numbers (#137) (*) | | | | | D TE | A |
| Frontiers in Chromatin Biology & Chemical Epigenetics/Epigenomics (#151) (*) | | D TE | DE | A | | |
| Fluorescent & Luminescent Proteins: New Chemistries & New Functions (#180) (*) | D | TA | | | | |
| Biomolecular Structure & Dynamics: Recent Advances in NMR (#181) (**) | | | DE | DE | TA | |
| Strategies for Coupling & Decoupling Diverse Molecular Units in the Glycosciences (#201) (*) | D | A | | | | |
| Enzyme Engineering & Biocatalysis Applications (#222) (**) | P | D TE | A | | | |
| Bioorganic Reaction Mechanisms (#224) (**) | | | PE | D | A | |
| Physiology & Metabolism of Extremophiles (#249) (*) | D TE | | | | | |
| Bio/chemical Approaches for Single-Cell Biosensing Technologies (#257) (*) | | | D | | | |
| Frontiers of Iron Chemistry in Biology (#268) (**) | D | A TE | | | | |
| Function, Chemistry & Signaling of Glycolipids & Phospholipids (#273) (**) | | | | D TE | | |
| Chemical Approaches to Astrobiology (#326) (*) | D | TA | | | | |
| Carbohydrate Recognition in Health & Disease (#342) (*) | D TE | D | | | | |
| Bioorthogonal Chemistry: Tools & Applications in Chemical Biology (#343) (*) | | D TE | D | | | |
| Chemistry & Applications of Retinal Proteins: From Microbes to Humans (#395) (*) | | | DE | A TE | | |

A = Oral AM P = Oral PM E = Oral Eve D = Oral AM/PM
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07. Biological (continued)

B I O L

| Sheraton Waikiki (*) & Royal Hawaiian (**) | T | W | T | F | S | S |
|---|---|----|---|----|---|---|
| Luciferin/Luciferase Engineering (#410) (*) | D | TE | | | | |
| Small-Molecule Interactions in Biomembranes (#418) (*) | | | D | TE | | |
| Chemical Biology of Protein-Lipid Modification (#421) (*) | D | TA | | | | |
| The RNA World: From Prebiotic Chemistry to the Emergence of Complexity (#449) (*) | D | TE | | | | |
| Biological General Posters | | | | TA | | |

08. Materials & Nanoscience

M T L S

| Hawaii Convention Center | T | W | T | F | S | S |
|---|---|---|---|----|----|---|
| Organic, Inorganic & Hybrid Nanoparticles: Synthesis, Characterization & Applications (#23) | | | P | DE | DE | A |
| Nanocrystal Synthesis, Characterization, Assembly & Applications (#34) | D | E | E | P | | |
| Chemistry & Applications of Graphene (#39) | | | P | D | D | A |
| Conjugated Polymers for Biological Applications (#43) | D | A | | | | |
| Nanowires: Synthesis, Fundamental Properties & Novel Device Applications (#51) | | | D | A | | |
| Metal-Oxo Clusters: Molecular Design from Monomers to Infinity (#79) | | | E | PE | DE | A |
| Two-Dimensional Nanosheets & Nanosheet-Based Materials: Synthesis, Characterization, Functionalization & Applications (#95) | P | D | A | | | |
| Luminescent Nanomaterials: Properties, Mechanisms & Applications (#101) | | | P | TA | D | A |
| Molecular Adsorption on Metallic Interfaces: Beyond the Cartoons (#102) | D | A | | | | |
| Design, Synthesis & Applications of Advanced Porous Materials (#111) | D | D | | | | |
| Development of Nano Devices & Nanotechnologies for Environmental Monitoring & Remediation (#124) | | | | D | TE | |
| Frontier & Perspectives in Molecular Spintronics (#127) | D | D | | | | |

08. Materials & Nanoscience (continued)

M T L S

| Hawaii Convention Center | T | W | T | F | S | S |
|--|---|----|----|----|----|----|
| Functional Molecular Materials & Devices (#128) | | | | DE | D | A |
| Applications of Ultrasound to Nanoscience (#150) | P | | D | A | | |
| Mechanically Responsive Materials (#153) | | | DE | TA | | |
| Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157) | D | D | | | | |
| Electrochemistry on Boron-Doped Diamond (BDD) Electrodes (#162) | D | TA | | | | |
| Natural to Nanosphere Lithographies: Two Decades of Self-Assembled Advanced Materials (#177) | A | TE | | | | |
| Current & Future Applications of Nanotechnology in the Oil Industry (#197) | | | D | | | |
| Janus Materials: Design, Fabrication & Properties (#210) | | | | D | TE | |
| Frontiers of Organic Porous Materials: Structures, Properties & Applications (#223) | D | D | A | | | |
| Carbon Nanotubes: Preparation, Characterization & Applications (#227) | | | TE | DE | DE | A |
| Advances in Bioinspired & Biomedical Materials (#245) | | | PE | DE | A | TA |
| Self-Organization of Membrane Systems (#259) | | | D | A | | |
| Nanomaterials for Nanomedicine (#289) | D | D | | | | |
| Challenge for Rare-Element-Free Functional Materials (#291) | | | | D | TE | A |
| Advanced Materials for Photonics & Electronics: Fundamentals & Applications (#308) | D | D | A | | | |
| Nitroxide Radicals: Synthesis & Functional Bio-/Nanomaterials (#309) | | | P | D | A | TE |
| Data Mining & Machine Learning Meets Experiment & First-Principles Simulation for Materials Discovery (#314) | P | D | | | | |
| Membranes & Nanotechnologies for Energy & Environment Applications (#317) | | | D | D | | |
| Ceramic Materials & Processing for Advanced Applications (#341) | | | D | A | | |
| Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346) | | | D | DE | A | TE |

PROGRAM SUMMARY

08. Materials & Nanoscience (continued)

| | M | T | L | S |
|--|---------|----------|----------|---------|
| Hawaii Convention Center | T | W | T | F |
| The Physical Structure, Function of Biological & Bioinspired Soft Matter (#347) | D | A TE | | |
| Fundamentals & Applications of Nanomaterials for Energy Technologies (#348) | | | P TE | D A |
| Multiscale & Synergistic Supramolecular Systems in Material & Biomedical Sciences (#357) | | | P TA | D A |
| Materials for the Mitigation of Chemical Hazards (#388) | TA | D | A | |
| Design of Innovative Photochromic Applications (#399) | | D TE | A | |
| Safety & Sustainability of Nanotechnology (#404) | D TE | | | |
| Single-Molecule Function & Measurements (#408) | D DE | TA | | |
| Advances in Organic Light-Emitting Diodes (#409) | D TE | D | | |
| The Frontiers of Geometrically Frustrated Magnetic Materials (#430) | E DE | | | |
| Synthesis, Structure & Functionalities of Ferroelectrics & Multiferroics (#432) | | | PE TA | DE A |
| Self-Assembled Biofunctional Nanomaterials (#433) | D DE | PE TA | | |
| Application of Luminescent Materials for Radiation Detection (#442) | | P TE | | |
| Self-Organization: Novel Mesogens & Applications (#447) | | | D TE | A |
| Materials & Nanoscience General Posters | | | | TA |

09. Chemistry of Clean Energy Conversion, Storage & Production

| | E | N | R | G |
|---|---------|---------|---------|---|
| Hyatt Regency Waikiki | T | W | T | F |
| Chemistry of Automotive Emission Control Catalysis: Current R&D & Future Challenges (#21) | D TA | | | |
| Integrated Biomass Refinery by Precisely Designed Heterogeneous Catalysts (#54) | | | D TE | A |
| Nano Catalysis for Clean Energy & Environmentally Friendly Chemical Production (#81) | D DE | E TA | E | E |

09. Chemistry of Clean Energy Conversion, Storage & Production (continued)

| | E | N | R | G |
|--|---------|---------|---------|--------|
| Hyatt Regency Waikiki | T | W | T | F |
| Progress Toward a Lignocellulosic Biorefinery (#144) | D TE | | | |
| Theory & Computation for Efficient Utilization of Energy & Resources (#163) | P TE | D | A | |
| Nanostructured Oxides for Energy Harvesting & Water Splitting (#171) | | | P TE | D A |
| Dynamical Processes of Light-Harvesting Surfaces (#178) | D A | TA | | |
| Water-Phase Catalysis for Energy & Chemicals Production (#182) | D TE | A | | |
| Current Status & Future Prospect of Polymer Electrolyte Fuel Cells (#188) | P TE | DE | A | |
| Artificial Photosynthesis: Photo-induced Water Splitting (#193) | | | D TE | A |
| Energy Storage in Chemical Bonds: Advances in Chemistry & Materials for Hydrogen Storage (#216) | | | D TE | |
| New Generation of Electrochemical Energy Storage & Conversion System: Materials, Interface & In Situ Techniques (#250) | P TA | P | D | |
| Nanoporous Materials for Renewable Energy & Sustainability (#266) | | | P TE | D A |
| Artificial Photosynthesis: Reduction of Carbon Dioxide (#271) | D TE | A | | |
| Artificial Photosynthesis: Bioinspired Chemistry for Solar Fuel Production (#278) | P TA | A | | |
| Homogeneous Catalysis Methodologies for the Upgrading of Biomass-Derived Molecules (#301) | P D | | | |
| Advances in Microwave Green Chemistry (#360) | | | D TE | A |
| Challenges in Second-Generation Biofuels: Processing, Stability & Usage (#378) | | D TE | | |
| Bridging Homogeneous & Heterogeneous Catalysis in Biorefining of Lignin (#405) | | | | P A |
| Global Strategies for Algal Biomass for Bioenergy & Biorefinery (#407) | | | D TE | D D |
| Chemistry of Clean Energy Conversion, Storage & Production General Posters | TA | | | |

A = Oral AM P = Oral PM E = Oral Eve D = Oral AM/PM
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10. Bench to Bedside: Chemistry of Health Care

H L T H

| Sheraton Waikiki (*) & Royal Hawaiian (**) | T | W | T | F | S | S |
|---|---|----|----|---|---|---|
| Oligonucleotide Therapeutics: From Base Pairs to Bedsides (#8) (*) | D | A | TA | | | |
| Chemistry for Development of Theranostic Radiopharmaceuticals (#11) (*) | | D | A | | | |
| De Novo Drug Design (#28) (*) | | | | D | | |
| Advances in Polymers for Medicine (#52) (*) | | | D | D | | |
| Academic Drug Discovery (#69) (*) | | | P | D | A | |
| Fragment-Based Lead Discovery (#145) (*) | D | DE | TA | | | |
| Small-Molecule Epigenetic Modulators (#146) (*) | | | | P | A | |
| In Vivo Chemical Strategies for Functional & Translation Studies of Biological Networks & Pathways (#212) (*) | | | | D | A | |
| Chemistry of Molecular Imaging (#215) (*) | | P | D | | | |
| New Antibacterial Agents (#236) (*) | P | D | | | | |
| Nutraceuticals & Functional Food Ingredients: Chemistry & Health (#285) (*) | | D | D | | | |
| Molecular Design in Medicine: Concept to Commerce (#295) (*) | | | | D | A | |
| Noncanonical Approaches to ¹⁸ F-labeling: New Frontiers in Stable Non-carbon-fluorine Bonds (#337) (*) | | | | D | | |
| Drug Conjugates: Approaches to Delivering Active Drugs to Where They Are Needed (#385) (*) | P | A | | | | |
| Cancer-Targeted Delivery of Therapeutics & Diagnostics (#393) (**) | | | | D | A | |
| Spectroscopic Tools for the Treatment of Cancer (#397) (**) | D | DE | | | | |
| Recent Advances in Microfluidics for Radiochemical Synthesis (#416) (*) | D | | | | | |
| Bench to Bedside: Chemistry of Health Care General Posters | | | TA | | | |

11. Connecting Chemistry to Society

S C T Y

| Hawaii Convention Center | T | W | T | F | S | S |
|--|---|----|----|----|---|---|
| Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy & Water (#113) | | | PE | D | A | |
| Technology & Assessment Strategies for Improving Student Learning in Chemistry (#132) | | | D | D | | |
| Educational Approaches To Help Students Connect Chemistry to World Issues of Sustainability & Climate (#149) | | | | | A | A |
| The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other & with Society (#173) | D | D | | | | |
| Effective Collaboration Strategies to Drive Innovation in Drug Discovery & Development (#179) | P | | | | | |
| Small Businesses Reaching Out for Market Share: Tool Kit & Success Stories (#185) | | | | D | | |
| Historical Evolution of the Chemical Community in the Countries of the Pacific Rim (#198) | | | | | P | A |
| Bioactive Natural Products & Public Health in the Pacific Rim: From Aquatic Dietary Supplements to Marine & Freshwater Toxins (#230) | D | TA | | | | |
| Green & Sustainable Chemistry Education for Tomorrow's Citizens of the World (#334) | | | TE | D | A | |
| Policies & Procedures Regarding Primary Research Data (#335) | | | | A | | |
| Chemistry Education: International & Multicultural Perspectives (#365) | D | A | | | | |
| Women in Chemistry: Changing the Face of Science (#382) | D | D | | | | |
| Advancing Sustainability: Catalyzing Interdisciplinary Scholarship for Green Chemistry (#383) | | | | | D | |
| Active & Inquiry Learning in the Chemistry Classroom & Laboratory (#443) | | | DE | TA | | |
| University-Industry Collaboration, Regulatory Environments & Commercialization of Emerging Technology (#453) | A | | | | | |
| Safety in the Academic Research Laboratory (#460) | D | TA | | | | |
| Connecting Chemistry to Society General Posters | | | | TA | | |

PACIFICHEM 2015

POSTER SESSIONS

Wednesday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|--|--|
| (1) Analytical | Innovation in Chemical Sensing and Separation Systems toward Advanced Chemical Analysis (#159) |
| (1) Analytical | Symposium on Petroleomics: Molecular Level Understanding of Petroleum for Environmental Science and Petroleum Engineering (#247) |
| (1) Analytical | (Bio-)Chemical / Electrochemical Sensors and Sensing Materials (#417) |
| (1) Analytical | Plasmonic Materials for Chemical Analysis (#450) |
| (1) Analytical | Analytical General Posters |
| (2) Inorganic | Dynamic Aspects of Solid Materials: From Equilibrium to Non-equilibrium Systems (#376) |
| (3) Macromolecular | NMR Spectroscopy of Polymers and Biobased Materials (#12) |
| (3) Macromolecular | Simulation of Polymers (#110) |
| (3) Macromolecular | Macromolecular General Posters |
| (4) Organic | Mechanochemistry and Solvent-free Synthesis (#322) |
| (4) Organic | Carbenes and Carbenoids in Organic Synthesis (#362) |
| (4) Organic | Organic General Posters |
| (5) Physical, Theoretical & Computational | Theory of Main Group Chemistry Beyond First Row (#183) |
| (5) Physical, Theoretical & Computational | Frontier Chemical Applications Using Accelerator Based Photon Sources (#414) |
| (5) Physical, Theoretical & Computational | Frontiers of Photon Upconversion Based on Triplet-triplet Annihilation (#420) |
| (6) Agrochemistry, Environmental, and Geochemistry | Application of Mass Spectrometry to Agrochemical Challenges (#72) |
| (6) Agrochemistry, Environmental, and Geochemistry | Genomics and Metabolomics for Phytochemical Research (#267) |
| (6) Agrochemistry, Environmental, and Geochemistry | Phytochemicals for Crop Protection: Discovery to Molecular Target (#358) |

Wednesday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|---|--|
| (6) Agrochemistry, Environmental, and Geochemistry | Sources, Fates and Risks from Consumer Product Ingredients in the Environment (#391) |
| (6) Agrochemistry, Environmental, and Geochemistry | Agrochemistry, Environmental, and Geochemistry General Posters |
| (7) Biological | Fluorescent and Luminescent Proteins: New Chemistries and New Functions (#180) |
| (7) Biological | Chemical Approaches to Astrobiology (#326) |
| (7) Biological | Chemical Biology of Protein-Lipid Modification (#421) |
| (8) Materials & Nanoscience | Electrochemistry on Boron-doped Diamond (BDD) Electrodes (#162) |
| (8) Materials & Nanoscience | Materials for the Mitigation of Chemical Hazards (#388) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Chemistry of Automotive Emission Control Catalysis: Current R&D and Future Challenges (#21) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Artificial Photosynthesis: Bio-inspired Chemistry for Solar Fuel Production (#278) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Chemistry of Clean Energy Conversion, Storage, and Production General Posters |
| (10) Bench to Bedside: Chemistry of Health Care | New Antibacterial Agents (#236) |
| (10) Bench to Bedside: Chemistry of Health Care | Drug Conjugates: Approaches to Delivering Active Drugs to Where they are Needed (#385) |
| (10) Bench to Bedside: Chemistry of Health Care | Spectroscopic Tools for the Treatment of Cancer (#397) |
| (11) Connecting Chemistry to Society | Bioactive Natural Products and Public Health in the Pacific Rim: From Aquatic Dietary Supplements to Marine and Freshwater Toxins (#230) |
| (11) Connecting Chemistry to Society | Safety in the Academic Research Laboratory (#460) |

Wednesday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--------------------|---|
| (1) Analytical | Fundamentals and Applications of Atomic Spectrometry (#160) |
| (1) Analytical | Magnetoanalytical Science: Separation, Characterization and Imaging (#320) |
| (2) Inorganic | Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65) |
| (2) Inorganic | Dioxygen Activation Chemistry of Metalloenzymes and Models (#339) |
| (2) Inorganic | Isotope Production--Providing Important Materials for Research and Applications (#363) |
| (3) Macromolecular | Synthetic Biopolymers (#37) |
| (3) Macromolecular | Characterization of Polymers and Polymer Assemblies in Solution (#172) |
| (3) Macromolecular | Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281) |
| (3) Macromolecular | Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319) |
| (3) Macromolecular | Polymers for Energy and Optoelectronic Devices (#361) |
| (4) Organic | Prospects for Flow Chemistry (#29) |
| (4) Organic | Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41) |
| (4) Organic | Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74) |
| (4) Organic | Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100) |
| (4) Organic | Practical Application of Basic Research on Molecular Recognition (#136) |
| (4) Organic | Homogeneous Gold Catalysis: Methods, Theories and Applications (#192) |
| (4) Organic | Supramolecular Chemistry at the Interface of Materials, Biology, and Medicine (#300) |
| (4) Organic | Fluorinations and Fluoroalkylations (#310) |
| (4) Organic | Nanomaterials as Catalysts for Green Chemistry (#313) |
| (4) Organic | Organic Solid-State Chemistry: Structure, Property & Reactivity (#398) |

Wednesday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--|---|
| (4) Organic | Cognizance of Endangered Elements for Organic Synthesis (#415) |
| (4) Organic | Photoredox Catalysis in Organic Synthesis (#440) |
| (4) Organic | Catalytic Multicomponent, Tandem and Cascade Reactions (#455) |
| (5) Physical, Theoretical & Computational | Ultrafast Intense Laser Chemistry (#35) |
| (5) Physical, Theoretical & Computational | New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems (#84) |
| (5) Physical, Theoretical & Computational | Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130) |
| (5) Physical, Theoretical & Computational | Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134) |
| (5) Physical, Theoretical & Computational | Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168) |
| (5) Physical, Theoretical & Computational | Latest Development of Advanced Vibrational Spectroscopy (#187) |
| (5) Physical, Theoretical & Computational | Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344) |
| (5) Physical, Theoretical & Computational | Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370) |
| (6) Agrochemistry, Environmental, and Geochemistry | Ferrites and Ferrates: Chemistry and Applications in Sustainable Energy and Environmental Remediation (#13) |
| (6) Agrochemistry, Environmental, and Geochemistry | Nanointerfaces and their Role in Environmental Systems and Processes (#86) |
| (6) Agrochemistry, Environmental, and Geochemistry | Sustainable Chemistry: Beyond the Bench (#103) |
| (6) Agrochemistry, Environmental, and Geochemistry | Chemistry and Biology of Auxin, Strigolactone and their Interactions (#107) |
| (6) Agrochemistry, Environmental, and Geochemistry | Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400) |

POSTER SESSIONS

Wednesday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|---|--|
| (7) Biological | Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151) |
| (7) Biological | Physiology and Metabolism of Extremophiles (#249) |
| (7) Biological | Frontiers of Iron Chemistry in Biology (#268) |
| (7) Biological | Luciferin/Luciferase Engineering (#410) |
| (7) Biological | The RNA World: From Prebiotic Chemistry to the Emergence of Complexity (#449) |
| (8) Materials & Nanoscience | Conjugated Polymers for Biological Applications (#43) |
| (8) Materials & Nanoscience | Molecular Adsorption on Metallic Interfaces: Beyond the Cartoons (#102) |
| (8) Materials & Nanoscience | Design, Synthesis and Applications of Advanced Porous Materials (#111) |
| (8) Materials & Nanoscience | Frontier and Perspectives in Molecular Spintronics (#127) |
| (8) Materials & Nanoscience | Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157) |
| (8) Materials & Nanoscience | Natural to Nanosphere Lithographies: Two Decades of Self-assembled Advanced Materials (#177) |
| (8) Materials & Nanoscience | Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223) |
| (8) Materials & Nanoscience | Nanomaterials for Nanomedicine (#289) |
| (8) Materials & Nanoscience | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| (8) Materials & Nanoscience | Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery (#314) |
| (8) Materials & Nanoscience | The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347) |
| (8) Materials & Nanoscience | Safety and Sustainability of Nanotechnology (#404) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Progress Toward a Lignocellulosic Biorefinery (#144) |

Wednesday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|---|---|
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Water-phase Catalysis for Energy and Chemicals Production (#182) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Artificial Photosynthesis: Reduction of Carbon Dioxide (#271) |
| (11) Connecting Chemistry to Society | The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other and with Society (#173) |
| (11) Connecting Chemistry to Society | Chemistry Education: International and Multicultural Perspectives (#365) |

Thursday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|----------------|---|
| (1) Analytical | Current Issues in Teaching Analytical Chemistry (#38) |
| (1) Analytical | Frontiers in Flow Injection Analysis and Related Techniques (#45) |
| (1) Analytical | Advances in Analytical Ion Mobility Separations (#61) |
| (1) Analytical | Immunoanalysis: Applications and Trends for Environmental Monitoring and Human Health (#94) |
| (2) Inorganic | Organo-Main Group Avenues toward Advanced Materials (#16) |
| (2) Inorganic | Molecular Catalysis of Water Splitting Reactions (#76) |
| (2) Inorganic | Frontiers of Organo-f-element Chemistry (#125) |
| (2) Inorganic | Electron Transfer and Electrochemistry of Inorganic and Organometallic Materials (#126) |
| (2) Inorganic | Non-covalent Interactions in Coordination Systems (#161) |

Thursday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|---|--|
| (2) Inorganic | Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186) |
| (2) Inorganic | Nuclear Probes in Nanoscale Characterization (#254) |
| (2) Inorganic | Metal-containing π-Conjugated Systems: Syntheses, Properties, Applications (#269) |
| (2) Inorganic | New Frontiers in Bioinorganic Chemistry (#356) |
| (3) Macromolecular | Polymer Gels as Advanced Soft Materials (#83) |
| (3) Macromolecular | Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112) |
| (3) Macromolecular | Functional Materials Based on Organic-inorganic Hybrid Polymers (#221) |
| (4) Organic | Molecular and Supramolecular Photochemistry (#71) |
| (4) Organic | Molecular Function of Natural Products: Advances towards Chemical Biology (#237) |
| (4) Organic | Frontiers of Chirality in Organic Chemistry (#286) |
| (5) Physical, Theoretical & Computational | Synergistic Relationships between Computational Chemistry and Experiment (#9) |
| (5) Physical, Theoretical & Computational | Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60) |
| (5) Physical, Theoretical & Computational | Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142) |
| (5) Physical, Theoretical & Computational | Frontiers of Plasmon Enhanced Spectroscopy (#428) |
| (5) Physical, Theoretical & Computational | Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438) |
| (5) Physical, Theoretical & Computational | Interplay between Chemistry and Dynamics in Biomolecular Machines (#441) |

Thursday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|--|--|
| (6) Agrochemistry, Environmental, and Geochemistry | UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204) |
| (7) Biological | Advances in Biological Solid-State NMR (#120) |
| (8) Materials & Nanoscience | Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23) |
| (8) Materials & Nanoscience | Nanocrystal Synthesis, Characterization, Assembly and Applications (#34) |
| (8) Materials & Nanoscience | Mechanically Responsive Materials (#153) |
| (8) Materials & Nanoscience | Single-Molecule Function and Measurements (#408) |
| (8) Materials & Nanoscience | Self-assembled Biofunctional Nanomaterials (#433) |
| (9) Chemistry of Clean Energy | Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81) |
| (9) Chemistry of Clean Energy | Dynamical Processes of Light Harvesting Surfaces (#178) |
| (9) Chemistry of Clean Energy | New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250) |
| (10) Bench to Bedside: Chemistry of Health Care | Oligonucleotide Therapeutics: From Base Pairs to Bedsides (#8) |
| (10) Bench to Bedside: Chemistry of Health Care | Fragment-based Lead Discovery (#145) |
| (10) Bench to Bedside: Chemistry of Health Care | Chemistry of Molecular Imaging (#215) |

POSTER SESSIONS

Thursday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--------------------|---|
| (1) Analytical | Supercritical Fluid Chromatography (SFC) for Analysis and Purification (#53) |
| (1) Analytical | On-site and In-vivo Instrumentation and Applications (#88) |
| (1) Analytical | Advances in FTIR Microspectroscopy: 3D Tomography to Nanoscale Imaging (#315) |
| (2) Inorganic | Functional Nanomaterials Based on Coordination Chemistry (#73) |
| (2) Inorganic | Coordination and Supramolecular Chemistry for Aqueous Metal Ion Separations (#97) |
| (2) Inorganic | Frontiers of Molecular Magnetism (#109) |
| (2) Inorganic | Transition Metal Complexes of N-Heterocyclic and Mesoionic Carbenes: Structure, Materials and Catalytic Applications. (#195) |
| (2) Inorganic | Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239) |
| (2) Inorganic | Novel Heme Proteins and Model Systems (#305) |
| (3) Macromolecules | New Perspectives of Synthetic and Biological Soft Matter (#57) |
| (3) Macromolecules | Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194) |
| (3) Macromolecules | New Perspectives of Bioplastics for Environmental Benign Materials (#396) |
| (3) Macromolecules | Advances in Precision Polymer Synthesis Using Reversible Deactivation Radical Polymerization (#401) |
| (4) Organic | Reactive Intermediates and Unusual Molecules (#7) |
| (4) Organic | Electrochemical Reactions and Mechanisms in Organic Chemistry (#104) |
| (4) Organic | The Science and Strategy of Pharmaceutical Process Chemistry: Adapting to Global Regulatory Development Guidance on Process Impurities (#242) |
| (4) Organic | Molecular Self-Assembly and Functional Organic Nanostructures (#263) |

Thursday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--|--|
| (4) Organic | Molecular Probes and Fluorophores for Biological Imaging (#280) |
| (5) Physical, Theoretical & Computational | Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44) |
| (5) Physical, Theoretical & Computational | Chemistry of Atmospheric Aerosols (#56) |
| (5) Physical, Theoretical & Computational | Self-organization in Chemistry (#165) |
| (5) Physical, Theoretical & Computational | Single-molecule Fluorescence Imaging (#208) |
| (5) Physical, Theoretical & Computational | Practical Strategies for Modeling Non-Covalent Interactions (#372) |
| (5) Physical, Theoretical & Computational | Structure and Spectroscopy of Linear Polyenes: Finite and Infinite (#456) |
| (6) Agrochemistry, Environmental, and Geochemistry | Analysis of Flavors in Specialty Asian Foods (#58) |
| (6) Agrochemistry, Environmental, and Geochemistry | Complex Mineral Growth and Dissolution Reactions: Collaborative Experimental and Computational Perspectives (#225) |
| (6) Agrochemistry, Environmental, and Geochemistry | Opportunities and Advancements in Rice Research and Aquaculture Research (#282) |
| (6) Agrochemistry, Environmental, and Geochemistry | Status and Trends of Persistent Organic Chemicals in the Environment (#402) |
| (7) Biological | New Platforms for Natural Products Discovery (#18) |
| (7) Biological | Characterization and Applications of Food Enzymes (#59) |
| (7) Biological | Enzyme Engineering and Biocatalysis Applications (#222) |
| (7) Biological | Carbohydrate Recognition in Health and Disease (#342) |
| (7) Biological | Bioorthogonal Chemistry: Tools and Applications in Chemical Biology (#343) |
| (7) Biological | Small Molecule Interactions in Biomembranes (#418) |
| (8) Materials & Nanoscience | Nanowires: Synthesis, Fundamental Properties and Novel Device Applications (#51) |

Thursday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|---|---|
| (8) Materials & Nanoscience | Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95) |
| (8) Materials & Nanoscience | Applications of Ultrasound to Nanoscience (#150) |
| (8) Materials & Nanoscience | Carbon Nanotubes: Preparation, Characterization and Applications (#227) |
| (8) Materials & Nanoscience | Self-organization of Membrane Systems (#259) |
| (8) Materials & Nanoscience | Membranes and Nanotechnologies for Energy and Environment Applications (#317) |
| (8) Materials & Nanoscience | Ceramic Materials and Processing for Advanced Applications (#341) |
| (8) Materials & Nanoscience | Design of Innovative Photochromic Applications (#399) |
| (8) Materials & Nanoscience | Advances in Organic Light-Emitting Diodes (#409) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Theory and Computation for Efficient Utilization of Energy and Resources (#163) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Challenges in Second Generation Biofuels: Processing, Stability, and Usage (#378) |
| (10) Bench to Bedside: Chemistry of Health Care | Advances in Polymers for Medicine (#52) |
| (11) Connecting Chemistry to Society | Green and Sustainable Chemistry Education for Tomorrow's Citizens of the World (#334) |

Friday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|---|--|
| (1) Analytical | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| (1) Analytical | Micro- & Nanofabricated Analytical Devices for Chemical, Biochemical & Biomedical Platforms (#129) |
| (1) Analytical | Ultrasensitive Assays for Proteins and Protein Modifications (#287) |
| (2) Inorganic | Telomeres and other G-quadruplex Structures as Targets for Metallodrugs (#459) |
| (2) Inorganic | Inorganic General Posters |
| (3) Macromolecular | New Frontiers in Polymer Crystallization (#96) |
| (5) Physical, Theoretical & Computational | Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218) |
| (5) Physical, Theoretical & Computational | Interplay between Theory and Experiment in Catalytic Research (#277) |
| (5) Physical, Theoretical & Computational | Physical, Theoretical & Computational General Posters |
| (7) Biological | Biosynthesis of Natural Products (#27) |
| (7) Biological | Bioorganic Reaction Mechanisms (#224) |
| (7) Biological | Biological General Posters |
| (8) Materials & Nanoscience | Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79) |
| (8) Materials & Nanoscience | Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101) |
| (8) Materials & Nanoscience | Advances in Bioinspired and Biomedical Materials (#245) |
| (8) Materials & Nanoscience | Multi-scale & Synergistic Supramolecular Systems in Material and Biomedical Sciences (#357) |
| (8) Materials & Nanoscience | Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432) |
| (10) Bench to Bedside: Chemistry of Health Care | Academic Drug Discovery (#69) |
| (10) Bench to Bedside: Chemistry of Health Care | Bench to Bedside: Chemistry of Health Care General Posters |

POSTER SESSIONS

Friday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|-------------------------------------|---|
| (1) Connecting Chemistry to Society | Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113) |
| (1) Connecting Chemistry to Society | Active and Inquiry Learning in the Chemistry Classroom and Laboratory (#443) |
| (1) Connecting Chemistry to Society | Connecting Chemistry to Society General Posters |

Friday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--------------------|--|
| (1) Analytical | Optical Waveguide Techniques for the Analyses of Materials and Interfaces (#164) |
| (1) Analytical | Advanced Analytical Applications and Technical Developments of Soft X-Ray Spectroscopy (#303) |
| (1) Analytical | Vibrational Spectroscopy: New Developments and Applications in Biological and Medical Sciences (#375) |
| (1) Analytical | Advances in Terahertz Spectroscopy and Imaging (#413) |
| (2) Inorganic | Chemistry and Application of Boron Clusters (#152) |
| (2) Inorganic | Current Trends and Interconnectivities Among Fundamental and Applied Inorganic Fluorine Chemistry (#156) |
| (2) Inorganic | Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170) |
| (2) Inorganic | The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NO _x Generation, Signaling and Reduction in Biological Systems (#371) |
| (3) Macromolecular | Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158) |
| (3) Macromolecular | Macromolecular Self-Assembly for Smart Biomaterials (#196) |
| (3) Macromolecular | Cyclic & Topological Polymers (#248) |
| (3) Macromolecular | Advanced Membrane Separations (#262) |

Friday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--|---|
| (3) Macromolecular | Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294) |
| (3) Macromolecular | Polymer Materials Performance, Degradation and Optimization (#369) |
| (4) Organic | Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25) |
| (4) Organic | Anion Receptors (#31) |
| (4) Organic | Natural Product-based Drug Discovery (#66) |
| (4) Organic | Molecular Containers (#99) |
| (4) Organic | Organic Reactions in Aqueous Media (#131) |
| (4) Organic | New Organosulfur Chemistry (#436) |
| (5) Physical, Theoretical & Computational | Advances in Quantum Monte Carlo (#80) |
| (5) Physical, Theoretical & Computational | Recent Advances in Dynamics of Confined Liquids (#123) |
| (5) Physical, Theoretical & Computational | Challenges in Plasmonic Photochemistry (#176) |
| (5) Physical, Theoretical & Computational | Recent Progress in Matrix Isolated Species (#199) |
| (5) Physical, Theoretical & Computational | Metal Ions and Protein Functions: Theoretical Models and Applications (#202) |
| (5) Physical, Theoretical & Computational | Dynamical Intermolecular Interactions for Biological Functions (#307) |
| (5) Physical, Theoretical & Computational | Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403) |
| (6) Agrochemistry, Environmental, and Geochemistry | Chemicals of Emerging Environmental Concern: A Global Perspective (#19) |
| (6) Agrochemistry, Environmental, and Geochemistry | Chemical Ecology Applied to Sustainable Agriculture (#105) |
| (6) Agrochemistry, Environmental, and Geochemistry | Fate and Risks of Nanoparticles in Aquatic and Terrestrial Environments (#220) |

Friday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|---|---|
| (6) Agrochemistry, Environmental, and Geochemistry | Proteomics and Metabolomics in Agricultural, Environmental, and Public Health Sciences (#264) |
| (6) Agrochemistry, Environmental, and Geochemistry | Analytical Development Relevant to Environmental Exposure and Effects (#288) |
| (6) Agrochemistry, Environmental, and Geochemistry | Advances in Functional Foods and Flavor Chemistry Research (#329) |
| (6) Agrochemistry, Environmental, and Geochemistry | Fukushima and Radiological Contaminated Environments World-wide: The Important Role of Environmental Chemistry and Radiochemistry in Remediation and Restoration (#374) |
| (6) Agrochemistry, Environmental, and Geochemistry | Radioactive Contaminants and Waste Management in the Environment (#390) |
| (7) Biological | Advances in Peptide and Protein Chemistry (#6) |
| (7) Biological | Heat Shock Proteins: The Next Target in the Disease Frontier (#91) |
| (7) Biological | Bio/chemical Approaches for Single Cell Biosensing Technologies (#257) |
| (8) Materials & Nanoscience | Chemistry and Applications of Graphene (#39) |
| (8) Materials & Nanoscience | Janus Materials: Design, Fabrication and Properties (#210) |
| (8) Materials & Nanoscience | Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials (#309) |
| (8) Materials & Nanoscience | Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346) |
| (8) Materials & Nanoscience | Fundamentals and Applications of Nanomaterials for Energy Technologies (#348) |
| (8) Materials & Nanoscience | Application of Luminescent Materials for Radiation Detection (#442) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Nanostructured Oxides for Energy Harvesting and Water Splitting (#171) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216) |

Friday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|---|---|
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Nanoporous Materials for Renewable Energy and Sustainability (#266) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Advances in Microwave Green Chemistry (#360) |
| (10) Bench to Bedside: Chemistry of Health Care | Nutraceuticals and Functional Food Ingredients: Chemistry and Health (#285) |
| (11) Connecting Chemistry to Society | Technology and Assessment Strategies for Improving Student Learning in Chemistry (#132) |

Saturday Morning

Kamehameha Halls I, II, and III (Convention Center)
10:00–12:00

| Area | Symposium |
|--|---|
| (1) Analytical | Development and Applications of Techniques for Electrochemical Analysis (#24) |
| (2) Inorganic | Inorganic Complexes for Solar Energy Harvesting (#256) |
| (2) Inorganic | Metal Mediated Polymerization (#292) |
| (2) Inorganic | Metal Coordination Sphere Design for Challenging Bond Transformations (#318) |
| (3) Macromolecules | Aggregation Induced Emission: Materials and Applications (#444) |
| (4) Organic | Recent Trends in Organocatalysis (#122) |
| (6) Agrochemistry, Environmental, and Geochemistry | Advanced Products from Lignin and Micro- or Nano-fibrillated Cellulose (#70) |
| (6) Agrochemistry, Environmental, and Geochemistry | Enzymes Essential to Biosphere Health: Bioremediation and Biogeochemical Cycling (#219) |
| (7) Biological | Biomolecular Structure and Dynamics: Recent Advances in NMR (#181) |
| (8) Materials & Nanoscience | Materials & Nanoscience General Posters |
| (10) Bench to Bedside: Chemistry of Health Care | Small Molecule Epigenetic Modulators (#146) |

POSTER SESSIONS

Saturday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|----------------|---|
| (1) Analytical | Direct and Mediated Bioelectrocatalysis for Biosensors and Energy Conversion Applications (#89) |
| (1) Analytical | Novel Analytical Probes for In Vivo Optical Functional Imaging (#115) |
| (1) Analytical | Marine and Freshwater Toxins: Detection, Structure, and Pharmacology (#138) |
| (1) Analytical | Paper-Based Analytical Devices for Point of Need Measurements (#213) |
| (1) Analytical | Analytical Laser-Induced Breakdown Spectroscopy (LIBS) for Hazards Analysis, Forensics, and Health (#379) |
| (1) Analytical | Bacterial Identification by Mass Spectrometry (#389) |
| (1) Analytical | Advances in Analytical Techniques for Effective Food Allergen Management (#394) |
| (1) Analytical | Organized Surfactant Assemblies in Chemical Analysis and Separation Science: Fifty Years Later (#457) |
| (2) Inorganic | Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42) |
| (2) Inorganic | Metal-Organic Frameworks: Synthesis, Properties and Applications (#50) |
| (2) Inorganic | From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62) |
| (2) Inorganic | Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications (#87) |
| (2) Inorganic | Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus, and Synthesis (#226) |
| (2) Inorganic | The Expanding Periodic Table: New Discoveries and Chemistry of the Heaviest Elements (#234) |
| (2) Inorganic | Advances in the Medicinal Applications of N-Heterocyclic Carbene Metal Complexes and Azolium Cations (#255) |
| (2) Inorganic | S-block Metal Chemistry (#304) |
| (2) Inorganic | Activation of Small Molecules by Electropositive Metals Related to Chemical Energy Conversion (#380) |
| (2) Inorganic | New Directions for Sensing Metals in Biology (#424) |

Saturday Evening

Kamehameha Halls I, II, and III (Convention Center)
19:00–21:00

| Area | Symposium |
|--|--|
| (3) Macromolecular | Dynamic, Reversible, and Self-healing Materials (#64) |
| (3) Macromolecular | Current Polyurethane Science (#133) |
| (4) Organic | New Green Techniques for Medicinal Chemistry (#148) |
| (4) Organic | Applications of C-H Functionalization (#169) |
| (4) Organic | Strategies and Tactics for Complex Molecule Synthesis (#174) |
| (4) Organic | Cooperative Cocatalysis with Two Different Metals (#270) |
| (4) Organic | Chemical Glycosylation: Methods and Mechanisms (#306) |
| (4) Organic | New Horizon of Process Chemistry by Scalable Reactions and Technologies (#426) |
| (4) Organic | Asymmetric Supramolecular Catalysis (#451) |
| (4) Organic | Synthetic Modulators of Protein-Protein Interactions (#461) |
| (5) Physical, Theoretical & Computational | Conformational Dynamics of Biomolecules and the Biomolecule-Solvent Interface (#98) |
| (5) Physical, Theoretical & Computational | Advances in Quantum Dynamics from Spectroscopy to Reactions (#384) |
| (5) Physical, Theoretical & Computational | Reactive Intermediates in Combustion and Atmospheric Chemistry (#419) |
| (5) Physical, Theoretical & Computational | Recent Experimental and Theoretical Advances in Studies of Liquid Interfaces (#437) |
| (6) Agrochemistry, Environmental, and Geochemistry | Human Exposure to Environmental Contaminants (#26) |
| (6) Agrochemistry, Environmental, and Geochemistry | Recycling of Polymeric Materials: Challenges and Perspectives (#36) |
| (6) Agrochemistry, Environmental, and Geochemistry | Chemistry of Integrated Water Treatment Systems for Halogenated Organics and Long-lived Radionuclides (#454) |
| (7) Biological | Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10) |
| (7) Biological | Homeostasis of Transition Metal Ions in Biological Systems (#47) |
| (7) Biological | Life at Small Copy Numbers (#137) |

Saturday Evening

Kamehameha Halls I, II, and III (Convention Center)

19:00–21:00

| Area | Symposium |
|---|---|
| (7) Biological | Function, Chemistry, and Signaling of Glycolipids and Phospholipids (#273) |
| (7) Biological | Chemistry and Applications of Retinal Proteins: From Microbes to Humans (#395) |
| (8) Materials & Nanoscience | Development of Nano Devices and Nanotechnologies for Environmental Monitoring and Remediation (#124) |
| (8) Materials & Nanoscience | Functional Molecular Materials and Devices (#128) |
| (8) Materials & Nanoscience | Challenge for Rare Element-free Functional Materials (#291) |
| (8) Materials & Nanoscience | Self-organization: Novel Mesogens and Applications (#447) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Integrated Biomass Refinery by Precisely Designed Heterogeneous Catalysts (#54) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Artificial Photosynthesis: Photo-induced Water Splitting (#193) |
| (9) Chemistry of Clean Energy Conversion, Storage, and Production | Global Strategies for Algal Biomass for Bioenergy and Biorefinery (#407) |
| (10) Bench to Bedside: Chemistry of Health Care | In Vivo Chemical Strategies for Functional and Translation Studies of Biological Networks and Pathways (#212) |
| (10) Bench to Bedside: Chemistry of Health Care | Molecular Design in Medicine: Concept to Commerce (#295) |
| (10) Bench to Bedside: Chemistry of Health Care | Cancer-Targeted Delivery of Therapeutics and Diagnostics (#393) |

STUDENT POSTER COMPETITION FINALISTS

Hawaii Convention Center, Kamehameha Exhibit Halls I, II & III
 ■ Tuesday, December 15, 12:00 Noon–2:00pm

Area 1 – Analytical

| | | |
|----|---|---|
| 1 | Microfluidic image-processing-based multipoint crystallization analysis. Aoi Akiyama | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 2 | Early detection of anti-asparaginase to significantly increase remission rate in acute lymphoblastic leukemia therapy. Alexandra Aubé | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| 3 | Design and synthesis of a novel chemical crosslinker for protein structure determination. Kayla Downey | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| 4 | Digital microfluidic platform for UV-Vis absorbance spectroelectrochemistry. Michael Dryden | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 5 | One-step modification and structuring of PDMS surfaces and its application in the bench-top fabrication of self-driven microfluidic channels. Ayodele Fatona | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 6 | Optical nanoantenna for bacterial detection. Maho Fukuda | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| 7 | Development of protein concentration system based on pore-size control of molecular sieving gel by thermal-stimulus response. Yudai Fukushima | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 8 | Plasmonic nanoprobe for sensing hydrogen peroxide in living systems. Xin Gu | Plasmonic Materials for Chemical Analysis (#450) |
| 9 | Microfluidic single cancer cells isolation and analysis device by simple manual operation for cytoscreening of cancer stem cells. Yuya Hattori | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 10 | Asymmetric rhodamine-based fluorescence probes for multicolor in vivo imaging. Ryu Iwatate | Novel Analytical Probes for In Vivo Optical Functional Imaging (#115) |
| 11 | Novel nanofiber web-based dry electrodes for long-term biopotential monitoring. Lu Jin | (Bio-)Chemical / Electrochemical Sensors and Sensing Materials (#417) |
| 12 | Biomarkers research involved in salmonid diseases: An approach based on MALDI-MS coupled with data mining techniques. Xaviera López Cortés | Bacterial Identification by Mass Spectrometry (#389) |
| 13 | On-chip templated biosynthesis of unnatural and natural protein microarrays suitable for surface plasmon resonance imaging. Gerald Manuel | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| 14 | Evaluation of peptide-material interaction by force mapping method with an atomic force microscope. Masahito Mochizuki | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| 15 | Automatic assembly of non-spherical microscale particles using electroosmotic flow in a microfluidic device. Hiroko Moriyama | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 16 | Paper test card for quantifying beta-lactam antibiotics. Nicholas Myers | Paper-Based Analytical Devices for Point of Need Measurements (#213) |

Area 1 – Analytical

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| 17 | Evaluation of the intrinsic retention selectivity of hydrocarbonaceous and fluorocarbonaceous stationary phases by surface-bubble-modulated liquid chromatography. Keisuke Nakamura | Innovation in Chemical Sensing and Separation Systems toward Advanced Chemical Analysis (#159) |
| 18 | Parameters influencing the performance of inkjet-printed microfluidic paper-based analytical devices. Riki Ota | Paper-Based Analytical Devices for Point of Need Measurements (#213) |
| 19 | Analysis of neuronal cell with atomic force microscopy. Ikbum Park | New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15) |
| 20 | Current detection in microfluidic devices for measurement of cell deformability. Mamiko Sano | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 21 | Shear flow ice chromatography. Masaya Shimizu | Innovation in Chemical Sensing and Separation Systems toward Advanced Chemical Analysis (#159) |
| 22 | Methods for quantitative analysis of submerged solids for application to deep-sea LIBS. Tomoko Takahashi | Analytical Laser-Induced Breakdown Spectroscopy (LIBS) for Hazards Analysis, Forensics, and Health (#379) |
| 23 | Design of bright fluorescent polymers for bioassays. Yuka Takahashi | (Bio-)Chemical / Electrochemical Sensors and Sensing Materials (#417) |
| 24 | Fluorescence polarization imaging for analyzing molecular interactions. Osamu Wakao | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 25 | Transportation imaging of exosomes derived from stem cells and cancer cells. Asami Yokoyama | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |
| 26 | Formation of the SERS-active substrate and its application in catalysis and analytical detection. Jingjing Zhao | Development and Applications of Techniques for Electrochemical Analysis (#24) |
| 27 | NAIMS: Nanotip ambient ionization mass spectrometry. Zhenpeng Zhou | Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129) |

Area 2 – Inorganic

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|----|--|---|
| 28 | Synthesis and study of novel iron sulfide complexes as models for nitrogenase. Nicholas Arnet | Metal Coordination Sphere Design for Challenging Bond Transformations (#318) |
| 29 | Exploration of new anionic selenium based pincer ligands. Bronте Charette | Inorganic General Posters |
| 30 | Homoleptic Au(III) trications: A synthetic pathway to a novel class of Au(III) compounds. Robert Corbo | Metal Coordination Sphere Design for Challenging Bond Transformations (#318) |
| 31 | Synthesis, characterization, and unique catalytic activities of a fluorinated nickel enolate. Ryohei Doi | Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186) |
| 32 | Ligand cooperation in the hydrogenation of N ₂ O using PCP iridium pincer complexes. Lauren Doyle | Metal Coordination Sphere Design for Challenging Bond Transformations (#318) |
| 33 | Synthesis and catalytic activity of dimolybdenum-dinitrogen complex bearing PCP-type pincer ligands. Aya Eizawa | Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170) |
| 34 | Redox active ligands: Ligand-centered electrocatalytic proton reduction and hydrogen oxidation. Andrew Haddad | Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications (#87) |
| 35 | 2:1 Coupling of terminal alkynes with secondary amines catalyzed by quinolinolato rhodium complexes. Moe Hamada | Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186) |
| 36 | P-C bond oxidation via Baeyer-Villiger mechanism. Gordana Ilic | Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus, and Synthesis (#226) |
| 37 | Optical responses of octanuclear gold clusters modifying thiolate ligands. Mitsuhiko Iwasaki | Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239) |

Area 2 – Inorganic

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| 38 | Synthesis and structure of ladder-type Pd-halide chain complex. Ryohei Kimura | Functional Nanomaterials Based on Coordination Chemistry (#73) |
| 39 | Revival of frustrated Lewis pairs from shelf-stable complexes comprised of borane and N-phosphine oxide substituted imidazolylidene. Takuya Kinoshita | Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65) |
| 40 | Polysilane confined in coordination nanospaces. Takashi Kitao | Functional Nanomaterials Based on Coordination Chemistry (#73) |
| 41 | N ₂ -splitting and functionalization in the coordination sphere of rhenium. Isabel Klopsch | Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170) |
| 43 | Studies on electrochemical hydrogen evolution from water catalyzed by bis(dithiolato)nickelate(II) complexes. Keita Koshiba | Molecular Catalysis of Water Splitting Reactions (#76) |
| 44 | Cooperative small molecule activation at the nickel-carbon double bond of nickel PCcarbeneP pincer complexes. Etienne LaPierre | Metal Coordination Sphere Design for Challenging Bond Transformations (#318) |
| 45 | Large spin-crossover [Fe ₄ L ₄] ⁸⁺ tetrahedral cage. Li Li | Functional Nanomaterials Based on Coordination Chemistry (#73) |
| 46 | Reaction dynamics for the C-H bond activation by iron(IV)-oxo complexes: Natural vs. biomimetic systems. Binh Mai | New Frontiers in Bioinorganic Chemistry (#356) |
| 47 | Ferrocenyl phosphonium cations as synthetically facile Lewis acids in organocatalysis. Ian Mallov | Inorganic General Posters |
| 48 | Copolymerization of ethylene with methyl acrylate by bisphosphine monoxide-palladium catalysts enabled by ligand-controlled insertion regioselectivity. Yusuke Mitsushige | Metal Mediated Polymerization (#292) |
| 49 | Effect of 5-aminolevulinic acid on cytochrome P450-based prodrug activation. Mai Miura | New Frontiers in Bioinorganic Chemistry (#356) |
| 50 | Electrocatalytic activation of CO ₂ by a series of rhenium complexes. Kankana Mullick | Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170) |
| 51 | Copolymerization of olefins and polar monomers by Pd/IzQO catalysts. Ryo Nakano | Transition Metal Complexes of N-Heterocyclic and Mesoionic Carbenes: Structure, Materials and Catalytic Applications. (#195) |
| 52 | Hydrogen ion beam irradiation effects on ZnO thin films studied by in-situ variable-temperature electrical resistivity measurements. Ryo Nakayama | From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62) |
| 53 | Synthesis of a novel molecular gear having a germanium junction and its gear slippage. Kazuma Okamura | Organic-Main Group Avenues toward Advanced Materials (#16) |
| 54 | Synthesis and analysis of new graphitic carbon nitride analogs. Shota Okamura | Electron Transfer and Electrochemistry of Inorganic and Organometallic Materials (#126) |
| 55 | Effective photosensitized energy transfer of nonanuclear terbium clusters using methyl salicylate derivatives. Shun Omagari | Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239) |
| 56 | Basicity of non-solvated boryl anion: Deprotonation of benzene. Takuto Osato | Organic-Main Group Avenues toward Advanced Materials (#16) |
| 57 | Reactivity of a Ga/P-based frustrated Lewis pair. Josephine Possart | Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65) |
| 58 | Carbodicarbene complexes of ruthenium: highly active catalysts for the hydrogenation of olefins. Conor Pranckevicius | Transition Metal Complexes of N-Heterocyclic and Mesoionic Carbenes: Structure, Materials and Catalytic Applications. (#195) |
| 59 | Toward C-H activation of hydrocarbons by rare earth NHC-complexes. Julia Rieb | Frontiers of Organo-f-element Chemistry (#125) |
| 60 | M ₂ L ₄ coordination cages as potential drug delivery systems for anticancer agents. Andrea Schmidt | New Frontiers in Bioinorganic Chemistry (#356) |
| 61 | Enhancing electrocatalytic hydrogen evolution by nickel molecular catalysts with the aid of Lewis acids in aqueous media. Hai Yan Shao | Molecular Catalysis of Water Splitting Reactions (#76) |

Area 2 – Inorganic

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| 62 | New approach to the fluorescence imaging of platinum drug processing. Clara Shen | New Frontiers in Bioinorganic Chemistry (#356) |
| 63 | Bright solid-state emission in disilane-bridged arenes including donor and acceptor moieties. Masaki Shimada | Organic-Main Group Avenues toward Advanced Materials (#16) |
| 64 | Electric conductive property of Hofmann-type coordination polymers including Pt-I chain pillars. Sayuri Shimoda | Metal-Organic Frameworks: Synthesis, Properties and Applications (#50) |
| 65 | Rare earth metal-mediated group transfer polymerization of vinylphosphonates: Tuning the metal ligand interaction via steric crowding at the rare earth center and novel highly efficient initiators from C-H bond activation. Benedikt Soller | Frontiers of Organo-f-element Chemistry (#125) |
| 66 | Characterization of a high-spin non-heme {FeN(H)O}8: Implications for the reactivity of iron nitroxyl species in biology. Amy Speelman | The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NOx Generation, Signaling and Reduction in Biological Systems (#371) |
| 68 | Harnessing weak interactions toward the synthesis of highly birefringent coordination polymers. John Thompson | Non-covalent Interactions in Coordination Systems (#161) |
| 69 | Photofunctional 1D coordination polymer based on bis(dipyrrinato) zinc(II) complex. Ryojun Toyoda | Inorganic General Posters |
| 70 | Synthesis and reactivity of neutral diborenes – the alkene analogs. Stefan Ullrich | Organic-Main Group Avenues toward Advanced Materials (#16) |
| 71 | Z-scheme photosynthesis for H2 evolution from water forming a three-electron-reduced species. Keiya Yamamoto | Molecular Catalysis of Water Splitting Reactions (#76) |
| 72 | Synthesis of multinuclear manganese complexes having a cage-type ligand: Structural models of oxygen evolving center. Shuhei Yonaga | Molecular Catalysis of Water Splitting Reactions (#76) |
| 73 | Direct visualization of guest dynamic behaviors in ultramicroporous crystal for exceptional thermal expansion. Hao-Long Zhou | Metal-Organic Frameworks: Synthesis, Properties and Applications (#50) |

Area 3 – Macromolecular

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| 74 | Cyclic carbonate as building block for sustainable synthesis of non-isocyanate polyurethane elastomers. Goliath Beniah | Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281) |
| 75 | Ultrabright organic dots with aggregation-induced emission characteristics for cell tracking. Xiaolei Cai | Aggregation Induced Emission: Materials and Applications (#444) |
| 76 | Aromatic end-group functionalization as a method to improve mechanical properties of poly(lactic acid). Love-Ese Chile | Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281) |
| 77 | Tough, thermoresponsive hydrogels. Jasmine Cubuk | Macromolecular General Posters |
| 78 | Preparation of glucose-responsive shape-memory hydrogels using molecular complexes as dynamic crosslinks. Masayoshi Hayashi | Polymer Gels as Advanced Soft Materials (#83) |
| 79 | Copolymerization of epoxides with CO2 catalyzed by multinuclear cobalt complexes. Yo Hirano | Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281) |
| 80 | Development of high thermoresistance and transparent polyurea films bioderived from 4-aminocinnamic acid. Yusuke Ibuki | Synthetic Biopolymers (#37) |
| 81 | Macroscopic artificial muscle powered by the microscopic sliding motion of [c2]daisy chain. Kazuhis Iwaso | Polymer Gels as Advanced Soft Materials (#83) |
| 82 | Ring-expansion living cationic polymerization: precision synthesis of ring-based functional polymers. Hajime Kammiyada | Cyclic and Topological Polymers (#248) |
| 83 | Synthesis of graft copolymers and dendronized polymers by Cu-catalyzed multicomponent polymerization. Hyunseok Kim | Macromolecular General Posters |
| 84 | Hydrogel with a reliable deformation region in an aqueous environment. Shinji Kondo | Polymer Gels as Advanced Soft Materials (#83) |

Area 3 – Macromolecular

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| 85 | Evaluation of interaction for bioactive compounds with thermoresponsive polymer brush grafted on polystyrene monolith surfaces using capillary chromatography. Takuya Koriyama | Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194) |
| 86 | Stretchable and highly conductive polymer gels. Tomoaki Kubota | Polymer Gels as Advanced Soft Materials (#83) |
| 87 | Formation of dynamic biomolecular recognition sites in smart hydrogels by molecular imprinting and their recognition control. Yoshiaki Kuriu | Polymer Gels as Advanced Soft Materials (#83) |
| 88 | Substantial spatial heterogeneity and tunability of glass transition temperature observed with dense polymer brushes prepared by ARGET ATRP. Tian Lan | Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194) |
| 89 | Synthesis and mechanical properties of joint-linker gels with reversible redox sol-gel transition. Kazumasa Moriyama | Polymer Gels as Advanced Soft Materials (#83) |
| 90 | Synthesis and electrochemical properties of radical polymer containing anionic group for a high energy density organic secondary battery. Tomoaki Murata | Polymers for Energy and Optoelectronic Devices (#361) |
| 91 | Physical hydrogels based on multifunctional polyurethanes via ionic or acidic crosslinking. Mai-Thi Nguyen-Kim | Polymer Gels as Advanced Soft Materials (#83) |
| 92 | Control of iterative double monomer addition for sequence-controlled vinyl polymers. Kana Nishimori | Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158) |
| 93 | Organic-inorganic hybrid polymers based on nickel(II) complexes of Goedken's macrocycle. Joseph Paquette | Functional Materials Based on Organic-inorganic Hybrid Polymers (#221) |
| 94 | High performance ambipolar field-effect transistor based on diketopyrrolopyrrole and benzodithiophene copolymer with cyanovinylene linkage. Junmo Park | Polymers for Energy and Optoelectronic Devices (#361) |
| 95 | Synthesis and properties of boron/silicon bimetallic copolymers. Puhup Puneet | Functional Materials Based on Organic-inorganic Hybrid Polymers (#221) |
| 96 | Light-emitting polycyclic aromatic hydrocarbon synthesized by regioselective photocyclization and its application in optical waveguide. Zijie Qiu | Aggregation Induced Emission: Materials and Applications (#444) |
| 97 | Association behavior of bovine serum albumin with the PEO-PPO multi-block copolymer in water. Kazuaki Rikiyama | Characterization of Polymers and Polymer Assemblies in Solution (#172) |
| 98 | Aliphatic polycarbonates based on carbon dioxide, furfuryl glycidyl ether, and glycidyl methyl ether: Reversible functionalization and crosslinking. Markus Scharfenberg | Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281) |
| 99 | Polyfullerene electrodes for high power supercapacitors. Tyler Schon | Polymers for Energy and Optoelectronic Devices (#361) |
| 100 | Investigation of the mechanism underlying biointerface of self-assembled monolayers by surface force measurements. Taito Sekine | Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194) |
| 101 | Activating polymer production with spinach leaves. Siva Shanmugam | Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281) |
| 102 | Facile one-pot preparation of 2D structure based on polymer self-assembly. Suyong Shin | Characterization of Polymers and Polymer Assemblies in Solution (#172) |
| 103 | End group removal of switchable RAFT agents. Sarah Stace | Advances in Precision Polymer Synthesis Using Reversible Deactivation Radical Polymerization (#401) |
| 104 | All-organic supercapacitors using PEDOT/PSS as flexible electrodes. Hiromi Takezawa | Polymer Gels as Advanced Soft Materials (#83) |
| 105 | Self-oscillating vesicles: Spontaneous cyclic changes of supramolecular structures formed by synthetic diblock copolymers. Ryota Tamate | Polymer Gels as Advanced Soft Materials (#83) |
| 106 | Metal ion-responsive biodegradable hydrogels made of PEG-DNA copolymers. Shizuma Tanaka | Polymer Gels as Advanced Soft Materials (#83) |

Area 3 – Macromolecular

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| 107 | Rocking chair-type charge-discharge property of redox copolymers and polymer composites containing TEMPO and charge-neutralizing anion. Hiroshi Tokue | Polymers for Energy and Optoelectronic Devices (#361) |
| 108 | Synthesis and conformational analysis of a double-stranded helical foldamer. Takahide Tsuda | Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112) |
| 110 | Living cationic polymerization via degenerative chain transfer on C-S bond. Mineto Uchiyama | Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112) |
| 111 | Characterization and substrate specificity of a poly(lactate-co-3-hydroxybutyrate) depolymerase from soil bacterium. Camila Utsunomia | New Perspectives of Bioplastics for Environmental Benign Materials (#396) |
| 112 | Chiral crystals of inorganic-organic hybrids based on polyoxometallates and supramolecular cations. Jun Xiong | Functional Materials Based on Organic-inorganic Hybrid Polymers (#221) |
| 113 | Electrochemical characterization of polycarbonate-based electrolytes for all-solid-state Li batteries. Mari Yajima | Polymers for Energy and Optoelectronic Devices (#361) |
| 114 | Stimuli-responsive supramolecular assemblies of amphiphilic self-immolative polymers. Rebecca Yardley | Macromolecular Self-Assembly for Smart Biomaterials (#196) |

Area 4 – Organic

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| 115 | Metabolomics approach to study the effect of Andrographis paniculata in improving chemotherapy treatment in colon cancer. Soha Ahmadi | Natural Product-based Drug Discovery (#66) |
| 116 | Silicon analog of the smallest bridgehead alkene. Naohiko Akasaka | Reactive Intermediates and Unusual Molecules (#7) |
| 117 | Barbiturated naphthalenes with flexible oligo(ethyleneglycol) side chains. Keisuke Aratsu | Molecular Self-Assembly and Functional Organic Nanostructures (#263) |
| 118 | Unprecedented alkali metal amide-catalyzed formal C(sp ³)-H bond activation. Wei Bao | Applications of C-H Functionalization (#169) |
| 119 | Total syntheses of hyperforin, papuaforin A-C and formal synthesis of nemorosone: Toward the total synthesis of ginkgolides. Gabriel Bellavance | Homogeneous Gold Catalysis: Methods, Theories and Applications (#192) |
| 120 | Cooperative catalysis of Cu and Mn in aerobic oxidative coupling of terminal alkynes. Sourav Biswas | Cooperative Cocatalysis with Two Different Metals (#270) |
| 121 | U.V. light mediated synthesis of carbazoles using flow chemistry. Antoine Caron | Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74) |
| 122 | Functional poly(2-oxazoline)s possessing solvatochromic fluorescent pyrene dye and the development of fluorescent hydrogel. Chia-Hsiu Chen | Cognizance of Endangered Elements for Organic Synthesis (#415) |
| 123 | Light induced molecular machine: Ruthenocene-based supermolecular crystals. Kai Jen Chen | Molecular and Supramolecular Photochemistry (#71) |
| 124 | Regiochemistry-directed syntheses of polyhydroxylated alkaloids from chiral aziridine. Jihye Choi | Organic General Posters |
| 125 | Bioimaging of HER-2 specific affibody conjugated two-photon fluorescent probe for detection of breast cancer. Ji-Woo Choi | Molecular Probes and Fluorophores for Biological Imaging (#280) |
| 126 | Aldehyde-selective Wacker oxidations of allylic fluorides. Crystal Chu | Organic General Posters |
| 127 | Chemistry of tetra-, penta-, and hexacationic systems. Makafui Gasonoo | Reactive Intermediates and Unusual Molecules (#7) |
| 128 | Fate of NHC-stabilized dicarbon. Dayne Georgiou | Reactive Intermediates and Unusual Molecules (#7) |
| 129 | Synthesis and investigation of enzyme-triggered CO-releasing molecules for biological and pharmaceutical applications. Anna-Lena Göderz | Organic General Posters |

Area 4 – Organic

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| 130 | Five-membered ring construction via chain-walking cycloisomerization of various 1,n-dienes catalyzed by palladium complexes. Taro Hamasaki | Catalytic Multicomponent, Tandem and Cascade Reactions (#455) |
| 131 | Synthesis and NMR properties of H ₂ - and H ₂ O-encapsulating aza[60]fullerenes. Yoshifumi Hashikawa | Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41) |
| 132 | Development of the new firefly luciferin analog aiming at detection of a free radical in the living body. Shuji Ioka | Molecular Function of Natural Products: Advances towards Chemical Biology (#237) |
| 133 | Asymmetric autocatalysis triggered by helical arrangement of chiral crystals of achiral organic compounds. Yoshiyasu Kaimori | Frontiers of Chirality in Organic Chemistry (#286) |
| 134 | Shape-persistent cavities of a rigid dendrimer. Yuto Kato | Practical Application of Basic Research on Molecular Recognition (#136) |
| 135 | Synthesis and properties of binuclear paddlewheel-type complexes with azulene ligand. Reiya Kawano | Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25) |
| 137 | Pd-catalyzed asymmetric intermolecular addition of homopropargylic alcohol to alkoxyallene: Development and application. Jungjoon Kim | Homogeneous Gold Catalysis: Methods, Theories and Applications (#192) |
| 138 | Studies toward the total synthesis of pactamycin. Taejung Kim | Organic General Posters |
| 139 | Unified total synthesis of ryanoids. Masaki Koshimizu | Strategies and Tactics for Complex Molecule Synthesis (#174) |
| 140 | Enantioselective borylative dearomatization of indoles by copper(I) catalysis. Koji Kubota | Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100) |
| 141 | Visible light induced photocatalysis for C–H imidation of arenes and heteroarenes. Dong Gil Lee | Photoredox Catalysis in Organic Synthesis (#440) |
| 142 | Chiral phosphoric acid catalyzed 1,2-sulfur rearrangement/enantioselective nucleophilic addition of dithioketal derivatives. Feng Li | Recent Trends in Organocatalysis (#122) |
| 143 | New functionalization approaches for trimetallic nitride metallofullerenes. Tinghui Li | Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41) |
| 144 | α -Boryl aldoximes: Novel reagents for the synthesis of drug-like small molecules. Sean Liew | Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100) |
| 145 | Development of new synthetic reactions leading to organophosphorus compounds having chiral carbon centers. Yuuki Maekawa | Frontiers of Chirality in Organic Chemistry (#286) |
| 146 | Iron-catalyzed reaction of amides and alkynes via C–H bond activation. Tatsuaki Matsubara | Cognizance of Endangered Elements for Organic Synthesis (#415) |
| 147 | Development of hydroxyapatite-supported ruthenium-vanadium bimetallic catalyst for highly selective reduction of amides to amines. Kazuya Miyagawa | Cooperative Cocatalysis with Two Different Metals (#270) |
| 148 | Hierarchical construction of multistructural porous organic salts (POSSs) through different networks of supramolecular clusters. Tetsuya Miyano | Organic Solid-State Chemistry: Structure, Property & Reactivity (#398) |
| 149 | Nickel-catalyzed transformation involving the cleavage of a carbon–nitrogen bond in aniline derivatives. Keisuke Nakamura | Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100) |
| 150 | Solvent free chiral inversion of thalidomide and hydrolysis product of thalidomide. Miri Nakamura | Frontiers of Chirality in Organic Chemistry (#286) |
| 151 | Synthesis of extended π -conjugated molecules with phosphorus ring junctions via tandem phospha-Friedel–Crafts reaction. Soichiro Nakatsuka | Cognizance of Endangered Elements for Organic Synthesis (#415) |
| 152 | Synthesis and characterization of multinuclear Au complexes bridged by two 1,2,3-triazolylidene carbene-phosphine hybrid ligands. Masaki Nishimura | Carbenes and Carbenoids in Organic Synthesis (#362) |

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Area 4 – Organic

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| 153 | Development of transrepression-selective liver X receptor (LXR) ligands. Sayaka Nomura | Synthetic Modulators of Protein-Protein Interactions (#461) |
| 154 | Synthesis of boron-fused benzotetracene analogs via demethylative electrophilic C–H borylation. Misa Numano | Cognizance of Endangered Elements for Organic Synthesis (#415) |
| 155 | Morphological control of organic semiconductor crystals by surface design and matrix rheology. Satoshi Okada | Organic Solid-State Chemistry: Structure, Property & Reactivity (#398) |
| 156 | Total synthesis of Laurallene. Taku Okada | Strategies and Tactics for Complex Molecule Synthesis (#174) |
| 157 | Mechanochromic luminescence properties of D-A-D type dibenzo[a,j]phenazine derivatives. Masato Okazaki | Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25) |
| 158 | Total synthesis of conduramine D-1 via a highly regioselective and diastereoselective allylic amination using chlorosulfonyl isocyanate. Sook Jin Park | Natural Product-based Drug Discovery (#66) |
| 159 | Design and synthesis of solution processable, narrow band gap, near-IR absorbing small molecules. Abby-Jo Payne | Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25) |
| 160 | Metal-catalyzed amination processes in continuous flow synthesis. Henri Piras | Prospects for Flow Chemistry (#29) |
| 161 | Dehydration mechanism of Ciprofloxacin HCl and its implication to physicochemical properties. Okky Putra | Organic Solid-State Chemistry: Structure, Property & Reactivity (#398) |
| 162 | Identification of biosynthetic enzymes for MPIase, a glycolipozyme essential for membrane protein integration. Ryo Sato | Molecular Function of Natural Products: Advances towards Chemical Biology (#237) |
| 163 | Total syntheses of T988 B and C. Soichiro Sato | Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74) |
| 164 | Synthesis of quinoline-derived “archipelago model” asphaltene compounds via a multicomponent strategy. David Scott | Catalytic Multicomponent, Tandem and Cascade Reactions (#455) |
| 165 | CT complexes of unique molecular geometries from pincer-shaped pyrene donors and TCNQ. Yoshiki Shibuya | Organic Solid-State Chemistry: Structure, Property & Reactivity (#398) |
| 166 | Conversion of marine biomass to adipic acid. Nara Shin | Organic General Posters |
| 168 | Integration of aerobic oxidation of alcohols and unsaturated bond formation catalyzed by polymer-incarcerated metal nanoparticle catalysts. Aya Suzuki | Prospects for Flow Chemistry (#29) |
| 169 | Discovery of a potent and selective agonist of TRPA1 and direct observation of its binding to TRPA1 by electron microscopy. Junichiro Takaya | Molecular Function of Natural Products: Advances towards Chemical Biology (#237) |
| 170 | Toward the realization of “Molecular n-Bit Memory”: Preparation and dynamic redox behaviors of novel electron donors containing multiple dyrex units. Hitomi Tamaoki | Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25) |
| 171 | Synthesis of multisubstituted pyrroles via copper-catalyzed condensation of imines and diazocarbonyl compounds. Simon Tan | Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74) |
| 172 | Switching on elusive organometallic mechanisms with photoredox catalysis. Jack Terrett | Photoredox Catalysis in Organic Synthesis (#440) |
| 173 | Synthesis the planar chiral phosphine-olefin ligand base on the transition metal scaffold and application in asymmetric catalysis. Ya-Yi Tseng | Frontiers of Chirality in Organic Chemistry (#286) |
| 174 | Domino approach to dibenzopentafulvalenes by carbopalladation sequence. Jan Wallbaum | Organic General Posters |
| 175 | Synthetic challenges and characterization during the realization of polyyne metalloporphyrin complexes consisting of axial binding. Vroni Walter | Reactive Intermediates and Unusual Molecules (#7) |
| 176 | Cascading effect of copper in click reaction between radical species. Yuping Wang | Molecular Self-Assembly and Functional Organic Nanostructures (#263) |

Area 4 – Organic

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| 177 | Acceptorless dehydrogenation of alkanes through cooperative base metal catalysis. Julian West | Cooperative Cocatalysis with Two Different Metals (#270) |
| 178 | Total synthesis of apratoxin F. Li Xiao | Strategies and Tactics for Complex Molecule Synthesis (#174) |
| 179 | Host-guest complexation and TEM imaging of cyclodextrins on nanocarbon surface. Junya Yamada | Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41) |
| 180 | Photocatalyzed site-selective C-H/C-C conversion of functionalized alkanes. Keiichi Yamada | Applications of C-H Functionalization (#169) |
| 181 | E/Z-selective asymmetric conjugate addition to electron-deficient internal alkynes. Kohei Yamada | Recent Trends in Organocatalysis (#122) |
| 182 | Core-shell nanostructured Au@CeO ₂ catalyst for the highly selective semihydrogenation of alkynes to alkenes. Masaaki Yamamoto | Nanomaterials as Catalysts for Green Chemistry (#313) |
| 183 | Synthetic studies on ecteinascidin 743. Eiji Yoshida | Natural Product-based Drug Discovery (#66) |
| 184 | Supramolecular asymmetric photochirogenesis mediated by synthetic antibody: Ground- and excited-states interaction studies of synthetic antibody with 2-anthracenecarboxylate. Wijak Yospanya | Molecular and Supramolecular Photochemistry (#71) |

Area 5 – Physical, Theoretical & Computational

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| 185 | Electron-hole recombination in Sr-doped NaTaO ₃ photocatalysts: Solid-state synthesis vs. solvothermal synthesis. Longjie An | Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344) |
| 186 | Trapping a liquid micro-droplet in a vacuum toward wet chemistry of gas-phase clusters. Kota Ando | Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168) |
| 187 | Phase-modulated coherent spectroscopy applied to ultracold doped helium droplets. Lukas Bruder | Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370) |
| 188 | Excited state ab-initio molecular dynamics to model the green fluorescent protein photo-induced reactivity. Greta Donati | Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142) |
| 189 | Determination of absolute CEP of circularly-polarized few-cycle laser pulses by angle-resolved photoelectron spectra of tunnel-ionized photoelectrons. Shinichi Fukahori | Ultrafast Intense Laser Chemistry (#35) |
| 190 | SP Explorer: Novel software facilitating the exploratory analysis of chemical simulations. Kyle Hall | Synergistic Relationships between Computational Chemistry and Experiment (#9) |
| 191 | Development of a femtosecond laser-assisted electron scattering apparatus equipped with an angular-resolved time-of-flight analyzer. Kakuta Ishida | Ultrafast Intense Laser Chemistry (#35) |
| 192 | Influence of polarized light on metal nanoparticle-originating high resolution TIRF imaging. Ayumi Ishijima | Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134) |
| 193 | Laser trapping and fluorescence correlation spectroscopy for the study on viscosity of single supercooled water droplets in air. Tomoki Ishikawa | Chemistry of Atmospheric Aerosols (#56) |
| 194 | Single-molecule method for counting ligands associated with a conformational transition: Linking ion uptake to nucleic acid folding. David Jacobson | Deciphering Molecular Complexity from Single Molecules to Cellular Networks (#121) |
| 195 | Obtaining resolution enhanced fluorescence images and 3D orientation information of single molecules by polarization modulation. Laura Jess | Single-molecule Fluorescence Imaging (#208) |

Area 5 – Physical, Theoretical & Computational

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| 196 | Symmetric arrangements of xenon clusters and quantum vortices in helium nanodroplets. Curtis Jones | Quantum Fluid Clusters (#203) |
| 197 | Study on the structural change of WO ₃ in its photoexcited state using picosecond W L1-edge XANES. Daiki Kido | Frontier Chemical Applications Using Accelerator Based Photon Sources (#414) |
| 198 | Theoretical study on novel intermolecular interactions observed in gas-phase or liquid-phase conditions: Halogen bond, chalcogen bond, and their simple modeling by effective fragment potential. Nahoko Kuroki | Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438) |
| 199 | Systematic method to estimate solvation free energies from 2PT molecular dynamics. Hankyul Lee | Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60) |
| 200 | Location, location, location: Distance dependant plasmon-enhanced singlet oxygen generation. Nicolas Macia | Challenges in Plasmonic Photochemistry (#176) |
| 201 | Single-molecule piezoelectrics: A novel approach to energy harvesting materials. Christopher Marvin | Synergistic Relationships between Computational Chemistry and Experiment (#9) |
| 202 | Morphological diversity of giant vesicle-based protocell depending on degree of complexation of DNA and catalysts. Muneyuki Matsuo | Self-organization in Chemistry (#165) |
| 203 | Relativistic open-shell Hartree-Fock theory with time-reversal symmetry. Masahiko Nakano | Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130) |
| 204 | Use of 2D infrared spectroscopy for the quantification and spatial mapping of post-translation modifications of proteins. Lays Rezende Valim | Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370) |
| 205 | First-principles calculation of NMR shielding in paramagnetic molecules including magnetic couplings. Syed Awais Rouf | Physical, Theoretical & Computational General Posters |
| 206 | Electronic structure of a metal-organic super container molecule by single point DFT. Wendi Sapp | Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344) |
| 207 | Using 2DIR spectroscopy for label free analysis of drug protein interactions. Hugh Sowley | Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370) |
| 208 | Effects of the alkynyl substituents on the geometrical and electronic structures of “Magic-Number” Au ₁₃ cluster. Mizuho Sugiuchi | Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168) |
| 209 | Kinetic analysis for complex reaction networks: Application to organic reactions. Yosuke Sumiya | Synergistic Relationships between Computational Chemistry and Experiment (#9) |
| 210 | Molecular-level details of morphology-dependent exciton migration in poly(3-hexylthiophene) nanostructures. Patrick Tapping | Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44) |
| 211 | 2D white-light spectroscopy reveals exciton dynamics in next-generation solar cells. Martin Zanni | Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370) |

Area 6 – Agrochemistry, Environmental, and Geochemistry

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| 213 | Do differences in key amino acids in the aryl hydrocarbon receptor explain differences in sensitivity of fishes to dioxin-like compounds? Jon Doering | Environment and Gene Interaction (#336) |
| 214 | Simultaneous production of vitamin E and biodiesel from waste oils obtained during edible oil refining. Kousuke Hiromori | Sustainable Chemistry: Beyond the Bench (#103) |
| 215 | Removal of arsenic and lead from contaminated soils by washing with biodegradable chelating agents. Naoyuki Jii | Agrochemistry, Environmental, and Geochemistry General Posters |
| 216 | Biomonitoring persistent organic pollutants and emerging contaminants in breast milk from Korea. Sunggyu Lee | Human Exposure to Environmental Contaminants (#26) |

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| 217 | Effects of processing units on secondary metabolites and functional properties of carrot juice processing. Tingting Ma | Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400) |
| 218 | Covalent organic polymer functionalized activated carbon: A novel material for water contaminant removal and CO ₂ capture. Paul Mines | Chemistry of Integrated Water Treatment Systems for Halogenated Organics and Long-lived Radionuclides (#454) |
| 219 | Chemical ecology of fluorescent compounds in flower pollen. Shinnosuke Mori | Chemical Ecology Applied to Sustainable Agriculture (#105) |
| 220 | Phytotoxicity and insect antifeedant activity of calamenene and cadinene type sesquiterpenes from camphorweed exudate. Ryo Morita | Phytochemicals for Crop Protection: Discovery to Molecular Target (#358) |
| 221 | Fast, sensitive technique for real-time, <i>in situ</i> quantification of commonly applied pesticides in the atmosphere using high resolution time-of-flight chemical ionization mass spectrometry. Trey Murschell | Application of Mass Spectrometry to Agrochemical Challenges (#72) |
| 222 | Availability of woody biomass degraded by mushrooms as ingredient of fermented total mixed ration for feeding dairy cattle. Naoya Nagatani | Recycling of Polymeric Materials: Challenges and Perspectives (#36) |
| 223 | Pesticide residues and dietary risk assessment of pesticides in fruits and vegetables in Beijing, China from 2012 to 2014. Canping Pan | Human Exposure to Environmental Contaminants (#26) |
| 224 | Indium separation from lead-smelting dust by chelant-assisted extraction at high pressure and temperature. Hikaru Sawai | Agrochemistry, Environmental, and Geochemistry General Posters |

Area 7 – Biological

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| 225 | Titin-based fluorescent tension sensors reveal the mechanochemistry of focal adhesions. Kornelia Galior | Bio/chemical Approaches for Single Cell Biosensing Technologies (#257) |
| 226 | Raman imaging of <i>ex vivo</i> bone formation during osteoblast differentiation. Aya Hashimoto | Bio/chemical Approaches for Single Cell Biosensing Technologies (#257) |
| 227 | Synthetic study of the polymer as multivalent bioprobe (V): Novel approach for lectin detection using combination of the glycocluster effect and FRET in the fluorogenic glycopolymers. Riho Hayama | Carbohydrate Recognition in Health and Disease (#342) |
| 228 | Overcoming strand inhibition using viscous environments. Christine He | The RNA World: From Prebiotic Chemistry to the Emergence of Complexity (#449) |
| 229 | Membrane permeability and ion transport across the cell membranes induced by binol-functionalized ion transporters. Audrey Hébert | Small Molecule Interactions in Biomembranes (#418) |
| 230 | Functional and structural analyses of a c-di-GMP responsive riboswitch. Saki Inuzuka | Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10) |
| 231 | Artificial division of codon boxes to encode nonproteinogenic amino acids along with 20 proteinogenic ones. Yoshihiko Iwane | Advances in Peptide and Protein Chemistry (#6) |
| 232 | The forgotten heat shock protein, HSP27: The design and synthesis of molecules targeting HSP27 as chemotherapies. Jessica Kho | Heat Shock Proteins: The Next Target in the Disease Frontier (#91) |
| 233 | Developing novel photoaffinity probes to identify ‘readers’ of histone modifications. Xiao-Meng Li | Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151) |
| 234 | Influenza virus fusion peptide-induced membrane acyl chain hairpins detected by paramagnetic enhancement of ² H relaxation. Shuang Liang | Advances in Biological Solid-State NMR (#120) |
| 235 | Altering stability of a transmembrane protein, MsbA, by structural comparison with its thermophilic homolog. Ka Lu | Biological General Posters |
| 236 | Design and synthesis of peptidic probes for polycomb group proteins upregulated in stem cells and prostate cancer. Natalia Milosevich | Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151) |
| 237 | Genetic response against removal of CO from the blood of mice by an iron(II)porphyrin-cyclodextrin supramolecular complex. Saika Minegishi | Homeostasis of Transition Metal Ions in Biological Systems (#47) |

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| 239 | Characterization of the unusual enzymatic transformations in cylindrocyclophane biosynthesis. Hitomi Nakamura | Biosynthesis of Natural Products (#27) |
| 240 | Single cancer cell isolation on the microcavity array platform using photopolymerizable hydrogel. Ryo Negishi | Bio/chemical Approaches for Single Cell Biosensing Technologies (#257) |
| 241 | Molecular interaction between rhamnose and a bacteria recognition lectin. Sim Kun Ng | Carbohydrate Recognition in Health and Disease (#342) |
| 242 | Development of red-shifted luciferase mutants derived from Brazilian click beetle Pyrearinus termittluminans. Tomoki Nishiguchi | Luciferin/Luciferase Engineering (#410) |
| 243 | Study of synthetic membrane perturbing peptides incorporating crown-ether by oriented circular dichroism. Pierre-Alexandre Paquet-Côté | Small Molecule Interactions in Biomembranes (#418) |
| 244 | Combinatorial library screening platform for rapid discovery and SAR of protein ligands. Kevin Pels | Advances in Peptide and Protein Chemistry (#6) |
| 245 | Three-days rapid construction of artificial antibody libraries on T7 bacteriophages. Yumi Saigusa | Advances in Peptide and Protein Chemistry (#6) |
| 246 | Rhodopsin guanylyl cyclase of the aquatic fungus Blastocladiella emersonii enables fast optical control of cGMP signaling. Ulrike Scheib | Chemistry and Applications of Retinal Proteins: From Microbes to Humans (#395) |
| 247 | Probing [4Fe-4S] and nitrosyl chemistry with NRVS, Mössbauer, and EXAFS, for WhiD and NsrR proteins. Pauline Serrano | Frontiers of Iron Chemistry in Biology (#268) |
| 248 | Toward isoform-specific lipoxygenase inhibitors: Acetaminophen-inspired compounds. Ron Shah | Bioorganic Reaction Mechanisms (#224) |
| 249 | Application for live-cell imaging with chemically synthesized histone H2A. Takuma Sueoka | Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151) |
| 250 | Targeted labeling of glycans in B-cell lymphoma with CD22 ligands. Yuting Sun | Carbohydrate Recognition in Health and Disease (#342) |
| 251 | Analysis of the stability of DNA duplexes containing DNA damages. Masayo Suzuki | Bioorganic Reaction Mechanisms (#224) |
| 252 | Peptide-based tunable molecular wires. Georgina Sylvia | Advances in Peptide and Protein Chemistry (#6) |
| 253 | Synthetic genetic switches for directed differentiation of human pluripotent stem cells. Junichi Taniguchi | Biological General Posters |
| 254 | Engineering of Photobacterium Lipolyticum M37 lipase to increase catalytic activity for efficient production of biodiesel. Kyung Seok Yang | Enzyme Engineering and Biocatalysis Applications (#222) |

Area 8 – Materials & Nanoscience

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| 255 | Control of conjugated polymer nanoparticle size and emission properties through microfluidics synthesis. Thais Abelha | Conjugated Polymers for Biological Applications (#43) |
| 256 | Effects of resonant bonding in Sn ₂ Sb ₂ Se ₅ phase change materials. Min Ahn | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| 257 | Dielectric/electric properties of composites filled with multiwalled carbon nanotubes. Juras Banys | Carbon Nanotubes: Preparation, Characterization and Applications (#227) |
| 258 | Mesoporous silica nanoparticles: Promising theranostic nanocarriers to overcome current limitations in the treatment of cancer and neurodegenerative disease. Meryem Bouchoucha | Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23) |
| 259 | Nanograined half-Heusler TiNiSn for thermoelectric applications. Malinda Buffon | Fundamentals and Applications of Nanomaterials for Energy Technologies (#348) |
| 260 | Self-optimizing and template-free growth of nanopatterned semiconductor light absorbers in response to spectral illumination. Azhar Carim | Natural to Nanosphere Lithographies: Two Decades of Self-assembled Advanced Materials (#177) |

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| 261 | Molybdenum disulphide based nanocomposite material synthesis, characterisation, and sensing applications. Rhiannon Clark | Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95) |
| 262 | Combined total scattering and density functional theory studies of amorphous indium gallium zinc oxide. Dylan Fast | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| 264 | Polyoxometalates to metal oxide thin film: the effect of protonation. Lauren Fullmer | Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79) |
| 265 | Structural characterisation of multimetallic nanoparticles using XAS. Ian Godfrey | Nanocrystal Synthesis, Characterization, Assembly and Applications (#34) |
| 266 | Palladium-based octopodal nanocrystals formed via copper-assisted growth. Meredith Hartley | Nanocrystal Synthesis, Characterization, Assembly and Applications (#34) |
| 267 | High speed synthesis of boron doped diamond by solution plasma. Ryota Hishinuma | Electrochemistry on Boron-doped Diamond (BDD) Electrodes (#162) |
| 268 | Biomimetic water and oil selective open capillary prepaed by surface modification. Shuto Ito | Advances in Bioinspired and Biomedical Materials (#245) |
| 269 | Novel route for surface modification of superparamagnetic nanoparticles in suspension for biomedical applications. Dagmara Jaskolska | Nanocrystal Synthesis, Characterization, Assembly and Applications (#34) |
| 270 | Unraveling orientation distribution and merging behavior of monolayer MoS ₂ domains on sapphire. Qingqing Ji | Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95) |
| 271 | Electrical biosensor with nanomesh silicon channel via block copolymer lithography. Hyeong Min Jin | Materials & Nanoscience General Posters |
| 272 | Correlations between magnetism and conductivity in quasi-one-dimensional π -d molecular conductors (DIETSe) ₂ FeBr ₄ xCl _{4(1-x)} . Genta Kawaguchi | Functional Molecular Materials and Devices (#128) |
| 273 | Role of cross links on collagen fibril orientation in pericardium. Hanan Kayed | The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347) |
| 274 | Microbial encapsulation in alginate/polydopamine core/shell microbeads. Beom Jin Kim | Advances in Bioinspired and Biomedical Materials (#245) |
| 275 | High frequency tunable property of Ba(ZrxTi1-x)O ₃ films grown by reactive sputtering. Jinwoong Kim | Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432) |
| 276 | Developmental responses of hippocampal neurons on various functionalized surfaces. Mi-Hee Kim | Advances in Bioinspired and Biomedical Materials (#245) |
| 277 | Improved interface and CO ₂ permeability by dual-functional amphiphilic PDMS-g-POEM comb copolymer micelles. Sang Jin Kim | Materials & Nanoscience General Posters |
| 278 | Dynamic and mechanical manipulation of fluidic species using a hierarchical wrinkle structure. Toru Kimura | Functional Molecular Materials and Devices (#128) |
| 279 | Prediction of interface structure and energy with an aid of information science. Shin Kiyoohara | Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery (#314) |
| 280 | Nano-structured organic light emitting diode for suppression of roll-off characteristics toward electrically-pumped organic semiconductor laser diodes. Hiroyuki Kuwae | Advances in Organic Light-Emitting Diodes (#409) |
| 281 | Antimicrobial peptide stars: The road to discovery and development. Shu Jie Lam | Advances in Bioinspired and Biomedical Materials (#245) |
| 282 | Structural characterization of graphene based morphologies for cathode application in fuel cells. Karsten Lehmann | Chemistry and Applications of Graphene (#39) |
| 283 | CVD growth of large single crystal graphene. Li Lin | Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95) |

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| 284 | Novel method to fabricate anisotropic highly porous silica core/shell microspheres. Johannes Maisch | Janus Materials: Design, Fabrication and Properties (#210) |
| 285 | Li ₄ Ti ₅ O ₁₂ /Graphene nanoribbon composites as anodes for lithium-ion batteries. Phillip Medina | Fundamentals and Applications of Nanomaterials for Energy Technologies (#348) |
| 286 | Enhanced Immunostimulation for cancer vaccine with crosslinked CpG-ODN/β-1,3-glucan nanogel through hybridization. Noriko Miyamoto | Nanomaterials for Nanomedicine (#289) |
| 287 | Controlling the electronic properties of 2D MoS ₂ through thiol functionalization. Emily Nguyen | Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101) |
| 288 | Morphology control of polysaccharide composite hollow fibers using microfluidic techniques. Shun Ohyama | Advances in Bioinspired and Biomedical Materials (#245) |
| 289 | Ultra-conformable polymer nanosheets with inkjet-printed electric circuits. Marin Okamoto | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| 290 | Design of full-color thermally activated delayed fluorescence emitters based on benzonitrile derivatives and their application in organic light-emitting diodes. In Seob Park | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| 291 | On the utilization of anti-Stokes/Stokes ratios in single-molecule surface-enhanced Raman spectroscopy for nanoscale thermometry. Eric Pozzi | Single-Molecule Function and Measurements (#408) |
| 292 | Induced assembly of asymmetrically-functionalized gold nanoparticles using localized DNA hybridization. Lindsey Pruden | Janus Materials: Design, Fabrication and Properties (#210) |
| 293 | Detecting methylation in arginine using optical microresonators. Alejandra Rios | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| 294 | Nanoscale surface wrinkling in plant-based plywoods with hydration-induced chiral gradients. Pardis Rofouie | The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347) |
| 295 | Fabrication of ZnS-AgInS ₂ nanoparticles covering on SiO ₂ particles and characterization of their fluorescence property. Yusuke Saito | Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101) |
| 296 | High-energy lithium-sulfur batteries: From theoretical understanding to nanomaterials design. Zhi Wei Seh | Fundamentals and Applications of Nanomaterials for Energy Technologies (#348) |
| 297 | Study of new beryllium substituted langasites A ₃ Ga ₃ Ge ₂ BeO ₁₄ (A=Pr, Nd, Sm). Arzoo Sharma | The Frontiers of Geometrically Frustrated Magnetic Materials (#430) |
| 298 | Construction of chiral polyoxometalate/nanoparticle composites toward chirality transfer and enhancement. Lei Shi | Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79) |
| 299 | Thermal and electrical transport in template fabricated poly(3-hexylthiophene)-multiwalled carbon nanotube composite fibers. Matthew Smith | Nanowires: Synthesis, Fundamental Properties and Novel Device Applications (#51) |
| 300 | Biomolecular interactions at the biomolecule-PEDOT interface: Insights from first-principles calculations. Anas Sultan | Conjugated Polymers for Biological Applications (#43) |
| 301 | Room temperature synthesis of graphene - Mn ₃ O ₄ composite using different solvent system for supercapacitor application. Syed Nizar Syed Abdulrahim | Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23) |
| 302 | Magnetic-plasmonic hybrid Ag@FeCo@Ag core@shell@shell nanoprobes for isolation of intracellular membrane vesicles. Mari Takahashi | Nanomaterials for Nanomedicine (#289) |
| 303 | Mechanized metal-organic frameworks. Lili Tan | Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223) |
| 304 | Development of a novel enzymatic nano-reactors as biodetoxification nanomedicine. Hengmin Tang | Nanomaterials for Nanomedicine (#289) |
| 305 | Preparation of hollow nanocapsules for effective delivery of cationic sonosensitizers. Ryoma Teranishi | Self-assembled Biofunctional Nanomaterials (#433) |
| 306 | Efficient delivery of nucleic acid medicines using pH responsive pyramidal DNA. Shuto Tokunaga | Nanomaterials for Nanomedicine (#289) |

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| 307 | Effect of crystallization of nonlinear optical dye in organic photorefractive composites: Enhanced photoconductivity and change of the density of states. Sho Tsujimura | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |
| 308 | Fluid dynamic slicing of super tensile carbon nanotubes. Kasturi Vimalanathan | Carbon Nanotubes: Preparation, Characterization and Applications (#227) |
| 309 | Poisson ratio of collagen fibrils under tension. Hannah Wells | Advances in Bioinspired and Biomedical Materials (#245) |
| 310 | Elastic flexibility in molecular crystals of metal complexes. Anna Worthy | Mechanically Responsive Materials (#153) |
| 311 | Roll-to-roll fabrication of conductive polymer nanosheets and their application as skin-contact electrodes. Kento Yamagishi | Functional Molecular Materials and Devices (#128) |
| 312 | Planar heterojunction perovskite solar cells using sequential vacuum deposition method for high stability and low-cost. Kohei Yamamoto | Ceramic Materials and Processing for Advanced Applications (#341) |
| 313 | Correlation of charge mobility with energetic disorder of host molecules in p-doped organic semiconductors. Seung-Jun Yoo | Advances in Organic Light-Emitting Diodes (#409) |
| 314 | Bench top fabrication of transferrable micro/nanostructured gold electrodes for stretchable sensors and electronics. Yujie Zhu | Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308) |

Area 9 – Chemistry of Clean Energy Conversion, Storage, and Production

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| 315 | Study of structural effects via anodic aluminum oxide as a novel inorganic separator for lithium ion batteries. Yong-keon Ahn | Nanoporous Materials for Renewable Energy and Sustainability (#266) |
| 316 | Pyrites for conversion batteries: The effects of cation chemistry on electrochemical performance. Megan Butala | New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250) |
| 317 | Selected metal disulfides for fast and stable Na ⁺ intercalation/de-intercalation. Jun Chen | New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250) |
| 318 | Suppression of aluminum corrosion in highly concentrated electrolyte. Ching-hua Chiang | Chemistry of Clean Energy Conversion, Storage, and Production General Posters |
| 319 | In vitro production of isoprenol using novel mevalonate pathway enzymes from thermoplasma acidophilum. Matthew Cummins | Chemistry of Clean Energy Conversion, Storage, and Production General Posters |
| 320 | Surface enhanced IR absorption spectro-electrochemistry of immobilized [NiFe] hydrogenase on graphene oxide/Au hybrid electrodes. Harnchana Gatemala | New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250) |
| 321 | Syntheses, structures, and properties of alkali and alkaline earth metal complexes with o-phenylenediamine. Junki Ishii | Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216) |
| 322 | Synthesis of a series of bismuth mixed anions compounds and their application to photocatalytic water splitting and photovoltaic systems. Hironobu Kunioku | Artificial Photosynthesis: Photo-induced Water Splitting (#193) |
| 323 | Improvement of photocatalytic activity of hybrids with ruthenium complexes and carbon nitride for CO ₂ reduction under visible light. Ryo Kuriki | Artificial Photosynthesis: Reduction of Carbon Dioxide (#271) |
| 324 | Electrochemical impedance spectroscopy and pH-dependent kinetics of α-Fe ₂ O ₃ ultrathin films for photoelectrochemical water splitting. Jonathon Moir | Nanostructured Oxides for Energy Harvesting and Water Splitting (#171) |
| 325 | Preparation of H-β zeolite-enwrapped Co/Al ₂ O ₃ Fisher-Tropsch catalyst for high isoparaffins selectivity. Hieu Nguyen | Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81) |

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| 326 | Free energy landscape of charge separation in organic disordered materials from first principles simulation. Katsuhiko Nishimura | Dynamical Processes of Light Harvesting Surfaces (#178) |
| 327 | Photoexcited carrier dynamics of double-layered PbS/CdS quantum dot sensitized solar cells characterized by transient absorption methods. Koki Sato | Dynamical Processes of Light Harvesting Surfaces (#178) |
| 328 | Does it have to be carbon? Metal anodes in microbial fuel cells and related bioelectrochemical systems. Igor Schmidt | New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250) |
| 329 | New cathode of high capacity and superior cyclability for Na-ion batteries: $\text{Na}[\text{Ni}_{0.4}\text{Fe}_{0.2}\text{Mn}_{0.4-x}\text{Tix}]\text{O}_2$. Xin Sun | Chemistry of Clean Energy Conversion, Storage, and Production General Posters |
| 330 | Catalytic combustion reaction on Mn-modified hexagonal YbFeO_3 . Ryohei Tada | Chemistry of Automotive Emission Control Catalysis: Current R&D and Future Challenges (#21) |
| 331 | Development of bimetallic Fe-Ni NPs supported on CeO_2 for hydrogen production from chemical hydrogen storage materials. Tomohisa Taga | Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216) |
| 333 | Photocatalytic conversion of CO_2 by H_2O over the rare-earth oxide-modified Ga_2O_3 . Hiroyuki Tatsumi | Artificial Photosynthesis: Reduction of Carbon Dioxide (#271) |
| 334 | Fabrication of Ta_3N_5 photoanodes for solar water splitting by thin film transfer process. Chizhong Wang | Artificial Photosynthesis: Photo-induced Water Splitting (#193) |
| 335 | Polymer design of sterically-protected anion exchange membranes. Andrew Wright | Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188) |
| 336 | Proton-coupled redox processes of tris- <i>o</i> -benzoquinodiimine Fe(II) complex. Risa Yamamoto | Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216) |
| 337 | Energy transfer between subunits of dimeric photosystem II monitored by femtosecond transient absorption spectroscopy. Yusuke Yoneda | Artificial Photosynthesis: Bio-inspired Chemistry for Solar Fuel Production (#278) |
| 338 | Photoelectrochemistry and surface science of doped hematite catalysts: from fundamental to applied research. Peng Zhao | Nanostructured Oxides for Energy Harvesting and Water Splitting (#171) |

Area 10 – Bench to Bedside: Chemistry of Health Care

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| 339 | Exploration of the mechanism of action and structure-activity relationship for a new class of quinazolinone antibiotics. Renee Bouley | New Antibacterial Agents (#236) |
| 340 | Rational design of novel spinogenic benzothiazoles for enhancing cognitive function. Jessica Cifelli | Academic Drug Discovery (#69) |
| 341 | PNIPAM nanospheres grafted to polypropylene fabric for thermally controlled release of bacteriophage. Hollie Hathaway | New Antibacterial Agents (#236) |
| 342 | Creation of the hypoxia-specific oligonucleotide therapeutics system with intracellular environment-responsive peptide ribonucleic acids (PRNAs): Synthesis and antisense activities of new type of chimeric PRNA-DNA derivatives containing phosphoramidate linkage in PRNA-DNA junction. Masahito Inagaki | Oligonucleotide Therapeutics: From Base Pairs to Bedsides (#8) |
| 343 | SBDD approach of the novel inhibitor of bacterial multidrug efflux transporter. Yuta Inoue | New Antibacterial Agents (#236) |
| 344 | Development of a virus-based stealth filament for cancer therapy. Karin Lee | Advances in Polymers for Medicine (#52) |
| 345 | Two-photon live imaging of osteoclastic bone resorption in living mice using pH-activatable fluorescence probe. Hiroki Maeda | In Vivo Chemical Strategies for Functional and Translation Studies of Biological Networks and Pathways (#212) |

Area 10 – Bench to Bedside: Chemistry of Health Care

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| 346 | Design of mechanically patterned hydrogel for directing organ bud self-formation. Yuko Shimokawa | Advances in Polymers for Medicine (#52) |
| 347 | Hyperpolarized ^{15}N tripodal tetramine derivatives as sensors of free Zn^{2+} ions in vivo. Eul hyun Suh | Chemistry of Molecular Imaging (#215) |
| 348 | Targeting bioactive chemical space with a small natural products library: Expanding diversity and predictability. Jacqueline von Salm-Fries | Academic Drug Discovery (#69) |
| 349 | Electron-transfer-based combination therapy of cisplatin with a molecular promoter for cancer treatment. Qinrong Zhang | Academic Drug Discovery (#69) |

Area 11 – Connecting Chemistry to Society

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| 350 | Reversible photo-induced liquefaction and crystallization of ionic azobenzene derivatives with photon energy storage characteristics. Keita Ishiba | Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113) |
| 351 | Hydrated ionic liquids as effective solvent of renaturation of aggregated recombinant cellulase expressed in <i>Escherichia coli</i> . Mayuko Kajiyama | Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113) |
| 352 | Suppression effect on insulin amyloid by the use of ionic liquids. Erika Yamaguchi | Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113) |
| 353 | Energy and climate change presentation in undergraduate introductory chemistry textbooks. Rachel Yoho | Educational Approaches to Help Students Connect Chemistry to World Issues of Sustainability and Climate (#149) |

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2-2-5 Sakaimachi Naka-ku, Hiroshima, 730-0853, Japan , 81 82 231 0540, fax: 81 82 231 1451, e-mail:info@watanabechem.co.jp. Amino Acid Derivatives and Reagents for Peptide Synthesis.

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101

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COMPANIES LISTED BY BROAD CATEGORY

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| Center for Sustainable Materials Chemistry | 128 |
| CONFLEX Corp. | 106 |
| CRC Press / Taylor & Francis Group | 216 |
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| Gaussian | 100 |
| International Biotechnology Symposium 2016 (AusBiotech Ltd) | 130 |
| Korean Chemical Society | 208 |
| Magritek Inc. | 309 |
| Mestrelab Research SL | 319 |
| Nanalysis Corp. | 405 |
| Research Square/American Journal Experts | 226 |
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| Schrodinger LLC | 118 |
| Thales Nano Inc. | 317 |
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| X-Ability Co., Ltd. | 127 |

Accessible Products

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| International Biotechnology Symposium 2016 (AusBiotech Ltd) | 130 |
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| International Biotechnology Symposium 2016 (AusBiotech Ltd) | 130 |
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| Anton Paar | 303 |
| Biotechnology Industry Organization | 107 |
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| Reaction Biology Corp. | 112 |
| Riogen Inc. | 507 |
| TCI America | 116 |
| Watanabe Chemical Industries, Ltd. | 101 |

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| Advion | 401 |
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| Biotechnology Industry Organization | 107 |
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| Hielscher Ultrasonics | 109 |
| IKA Works, Inc. | 129 |
| International Biotechnology Symposium 2016 (AusBiotech Ltd) | 130 |
| Japan Analytical Industry Co. Ltd. | 232 |
| Little Things Factory GmbH | 511 |
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| Milestone SRL | 407 |
| Nanalysis Corp. | 405 |

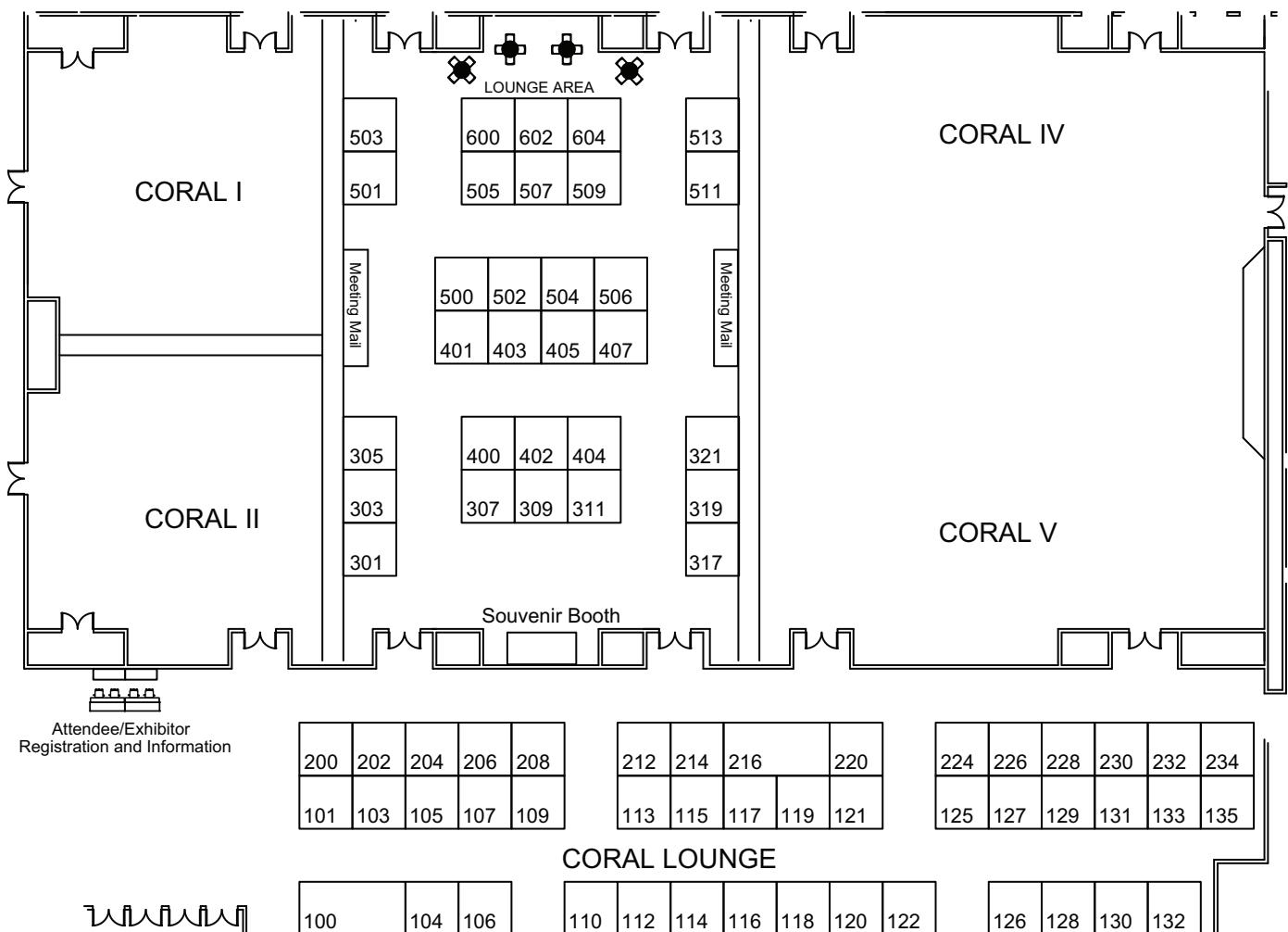
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| Parr Instrument Co. | 501 | Scientific Computer & Data Management | |
| Piercan USA Inc. | 500 | | |
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| Qorpak | 206 | CONFLEX Corp. | 106 |
| Reaction Biology Corp. | 112 | DeltaSoft Inc. | 125 |
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| Other | | JSOL Corporation | 321 |
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| ACS Publications | 200 | OpenEye Scientific Software | 121 |
| Center for Organic Photonics and Electronics Research, Kyushu University | 122 | Schrodinger LLC | 118 |
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| Mestrelab Research SL | 405 | Parr Instrument Co. | 501 |
| Nanalysis Corp. | 112 | PROTO Manufacturing | 404 |
| Reaction Biology Corp. | 507 | SpectroClick Inc. | 115 |
| Riogen Inc. | 118 | | |
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NEW PRODUCTS LISTING

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| Bio-Product 3DM protein superfamily system mutation prediction system | Booth # 114 | nanoplus Nanosystems and Technologies GmbH Booth # 307 DFB laser laser diode interband cascade laser quantum cascade laser |
| Biomatrik Inc mPEG Click PEGylation cross-linkers heterobifunctional | Booth# 504 | Parr Instrument Co. Booth # 501 6050 Compensated Calorimeter |
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| COSMOlogic GmbH & Co. KG COSMOtherm COSMOmic COSMOquick COSMOconf TURBOMOLE | Booth # 212 | Schrodinger LLC Booth # 118 Small Molecule Drug Discovery Suite Biologics Suite Materials Science Suite PyMOL |
| Gaussian Gaussian Gaussview AGUI GUI | Booth # 100 | Scientific Computing & Modelling NV Booth # 110 ADF2016 pre-release New ReaxFF analysis tools |
| Hielscher Ultrasonics Ultrasonic Homogenizer UIP2000hdT (2kW) SonoStep - Ultrasonic sample preparation Industrial Ultrasonicator UIP4000hdT (4 kW) Ultrasonic Lab Device UP200St (200W) Ultrasonic Probe Device UP200HT (200W) | Booth # 109 | TCI America Booth # 116 Lead(II) Iodide [for Perovskite precursor] 9-(3-Bromophenyl)carbazole Beclometasone Dipropionate Bis(trimethylsilylmethyl) Sulfide Carbinoxamine Maleate |
| Japan Analytical Industry Co. Ltd. Recycling Preparative HPLC/GPC Portable Pyrolyzer | Booth # 232 | University Science Books Booth # 402 Phys Chem for the Chem Sciences, Chang/Thoman X-Ray Crystallography, by Girolami Principles of NMR Spectroscopy, by Goldenberg Principles of Descriptive Inorg Chem, by Wulfsberg |
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| Korean Chemical Society Bulletin of the Korean Chemical Society Chemistry, An Asian Journal | Booth # 208 | Zaiput Flow Technologies Booth # 228 liquid-liquid separator back pressure regulator |

PACIFICCHEM EXPO 2015

December 15–20, 2015
Hilton Hawaiian Village
Honolulu, Hawaii



Plenary**Tuesday Evening**

Sheraton Waikiki
Hawaii Ballroom

Plenary Lecture

Presiding: P. Stang
19:00. The Disappearing Spoon. S. Kean

ANYL**Area 1 – Analytical****Tuesday Morning**

Marriott Waikiki Beach
Waikiki Blrllm III

New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15)

Organized by: S. Krylov, D. Wilson,
W. Zhong, H. Wang
Presiding: S. Krylov, W. Zhong

8:00 Opening remarks

8:05 – 1. Microscale thermophoresis: measuring biomolecule affinities by the molecule movement in a thermal gradient.
D. Braun

8:35 – 2. Kinetic separation: A conceptual platform for development of homogeneous kinetic affinity method.
S.M. Krylova, R. Yufa, J. Bao,
S. Beloborodov, M. Kanato

9:05 – 3. Selection of aptamers using a dual-partitioning approach. **S. Li**, J. Ashley,
K. Ji

9:25 – 4. Capillary electrophoresis-systematic evolution of ligands by exponential enrichment selection using modified nucleic acid libraries. **M. Kuwahara***

9:45 – 5. Multiple applications of CE in aptamers selection. **F. Qu***

10:05 Break

10:20 – 6. Novel designs for electrokinetic noncovalent interaction studies: An overview on powerful methodologies for the analysis of a wide range of chemical, biochemical, biological, and colloidal systems. G. Ramirez Garcia, F. d'Orlyé,
C. Perreard, **A. Varenne***

10:40 – 7. Chromatographic capillary electrophoresis (CCE): A method for kinetic study of intermolecular interaction.
K. Miyabe, Y. Shimazaki

11:00 – 8. New trends in affinity capillary electrophoresis (ACE) to study interactions in between biological macromolecules and drugs. **R.H. Neubert***

11:20 – 9. Study of protein-methylated DNA interaction by affinity capillary electrophoresis coupled laser-induced fluorescence. **H. Wang***

11:40 – 10. Therapeutic antithrombin: Molecular interaction studies based on affinity capillary electrophoresis and capillary electrophoresis-mass spectrometry.
M. Taverna*, A. marie, t. Tran-Maignan,
E.P. bianchini, D. Borgel, r. urbain,
j. Planter, F. Saller, G.W. Somsen,
E. DOMINGUEZ VEGA

Marriott Waikiki Beach
Milo III

Frontiers in Flow Injection Analysis and Related Techniques (#45)

Organized by: T. Imato, G. Christian,
K. Grupan, S. Kolev, A. Sabarudin

8:00 Opening Remarks
8:05 – 11. ICFIA history: Promoting international collaborations. **G.D. Christian***
8:30 – 12. Blueprint for the universal flow analyzer. **J. Ruzicka**

8:55 – 13. Online fractionation and determination of mercury in environmental solids using a sequential injection approach with atomic fluorescence detection.
Y. Zhang, M. Miro*, S.D. Kolev*

9:20 – 14. Enhanced chemiluminescence of peroxy nitrous acid by carbon nanoparticles and its application in flow injection analysis. **J. Lin, H. Chen, Z. Lin**

9:45 – 15. Measurement of octanol-water partition coefficient by zone fluidics.
D. Nacapricha*, P. Wattanasin,
P. Saeteer, P. Wilairat, S. Teerasong

10:00 Break

10:25 – 16. Conducting polymers for bacterial detection: Applications to sensors and trapping agents. D.Q. Le,
T. Kinoshita, A. Morishita, S. Tokonami,
T. Nishino, H. Shigui, **T. Nagaoka***

10:50 – 17. Monitoring of ppbv-level volatile sulfur compounds by continuous gas absorbing and miniaturized flow analysis method. **K. Toda***, S. Yunoki

11:15 – 18. Improvements in flow-injection NMR as a tool for high-throughput sample analysis. **P. Krolkowski***, S. Hollis,
R. Kautz, D. Strand

11:35 – 19. Flow-based chemical analysis using streams driven by centrifugal force. H. Tagami, R. Ishimatsu, K. Nakano,
Y. Chen, Z. Chen, P. Rattanarat,
P. Teengam, O. Chailapakul, **T. Imato**

Marriott Waikiki Beach
Kona Moku Blrllm C

Advances in Analytical Ion Mobility Separations (#61)

Organized by: A. Shvartsburg, F. Misaizu,
T. Pukala

Presiding: A. Shvartsburg

8:00 Introduction to Symposium

8:10 – 20. Stand-alone high resolution ion mobility spectrometer and its application in explosives detection and air monitoring. **H. Li***

8:40 – 21. Development of trap ion mobility system for separation. **T. Sugai***,
H. Yasuhiro, H. Matsubayashi,
R. Jinnochi

9:10 – 22. Ion collision cross section measurements in ion traps: Initial results.
W. Xu*, M. He, L. Mao

9:40 Break

10:00 – 23. Development of on-site hybrid instrument based on ion mobility spectrometry and arrayed electrochemical sensors against chemical warfare agents in vapor. **Y. Seto***, H. Nagashima,
T. Nagoya, T. Kondo, T. Satoh,
T. Ohmori, K. Tsuge, N. Nakano,
H. Sugiyama, T. Nishide, A. Ishizaki,
K. Daikuhara, Y. Kawahara, M. Kidera,
T. Urabe, H. Tanuma

10:30 – 24. Tandem ion mobility mass spectrometry – using light and collisions to change the shape of molecular ions.
B. Adamson, N. Coughlan, P. Markworth,
E. Bieske*

11:00 – 25. Novel approach for high IMS resolution using structures for lossless ion manipulations (SLIM). **Y.M. Ibrahim***,
A.M. Hamid, S.V. Garimella,
R.V. Norheim, G.A. Anderson, R.D. Smith

11:30 – 26. Characterising a t-wave enabled multi-pass cyclic ion mobility separator.
K. Giles*, R. Izuka

Marriott Waikiki Beach
Milo I

Immunoanalysis: Applications and Trends for Environmental Monitoring and Human Health (#94)

Organized by: S. Gee, I. Kennedy,
H. Ohkawa, T. Xu, T. Prapamontol

Presiding: T.-. Prapamontol

8:00 Introduction

8:05 – 27. Immunoassay, an alternative or complimentary technique to study pesticide contamination: A perspective from an environmental toxicology lab in Chiang Mai, Thailand. **T.-. Prapamontol***,
S.-. Hongsibsong, S. Thiphom, S. Gee,
B. Hammock

8:30 – 28. Role of immunoassay in human biomonitoring. **S. Gee**, B. Hammock

8:55 – 29. Immuno-analytical approach to the detection of endocrine disrupting chemicals in environment and food: Success, challenges, and limitations.
N.A. Lee*

9:20 – 30. Develop an ELISA kit to detect Endosulfan and cyclodien pesticides residues in agricultural products. **A.Q. Bui**

9:45 – 31. Highly specific fluorescence immunoassay developed for detection of di-isobutyl phthalate in edible oil samples.
S. Zheng, P. Wu, D. Lai, **S. Zhao**

10:05 Break

10:20 – 32. Development of an immunoassay and biosensor for the detection of the phenylpyrazole insecticide fipronil and its metabolite. **N. Vasyleva**, K. Ahn,
B. Barnych, S. Gee, B. Hammock*

10:40 – 33. Fast and sensitive detection of a neonicotinoid insecticide imidacloprid with a reagentless immunoassay reagent, Quenchbody. **J. Dong**, S. Zhao,
H. Jeong, K. Okumura, H. Ueda*

11:00 – 34. Biologically validating ELISAs for use in environmental monitoring of Cry proteins. **V.C. Albright**, R.L. Hellmich,
J.R. Coats*

Marriott Waikiki Beach
Kona Moku Blrllm A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree,
S. Jacobson, J. Ramsey, K. Otsuka,
D. Chung

Presiding: K. Otsuka

8:00 Introductory Remarks

8:05 – 35. High performance microscale liquid phase separations of biomolecules. Y. Fukushima, T. Naito, T. Kubo,
K. Otsuka*

8:30 – 36. Micro and extended-nano ELISA: Practical application and future.
T. Kitamori*

8:55 – 37. Stabilizing nanoporous structures for biomolecule separation. **J. Harrison***,
N. Shaabani, M. Azim, Y. Zhou,
A. Jemere

9:20 – 38. Novel solid-phase microextraction and capillary electrochromatographic column techniques for pharmaceutical analysis. **Z. Chen***

9:45 Break

10:00 – 39. Rapid isolation of circulating tumor cells with microfiber fabric and vacuum system. **M. Takai**

10:25 – 40. Application of nanoplasmonics-based microfluidic sensors for highly sensitive biomarker detection. **J. Choo***

10:50 – 41. Spatiotemporal control of biosensing by electrochemical lithography. **M. Nishizawa**

11:15 – 42. Unique separations for aromatic compounds by a C₆₀-fullerene bonded silica-monolithic capillary in liquid chromatography. **T. Kubo***, M. Tsuzuki,
T. Naito, K. Otsuka

11:30 – 43. Urinary iodine status determination by capillary electrophoresis: A robust assay for continuous monitoring of iodized salt programs for epidemiological studies. **P. Britz-McKibbin***,
A. Nori de Macedo

11:45 – 44. Low-aspect-ratio micropore sensors: possibilities and limitations.
M. Tsutsui*, A. Arima, K. Yokota,
M. Taniguchi, T. Kawai

Marriott Waikiki Beach
Milo IV / V

Innovation in Chemical Sensing and Separation Systems toward Advanced Chemical Analysis (#159)

Organized by: T. Hayashita, P. Dasgupta,
B. Cho, A. Tong, T. Okada, W. Zhong,
H. Li, H. Chang

Presiding: T. Hayashita, W. Zhong

8:00 Session Introduction

8:05 – 45. Electrophoretic separation of single molecules using thermoplastic nanocolumns. **S.A. Soper***

8:35 – 46. Single bubble microextraction coupled with capillary electrophoresis. S. Cho, **D. Chung***

8:55 – 47. Microfluidic systems integrating on-chip sample preparation with capillary electrophoresis. **A.T. Wooley***,
S. Kumar, M. Sonker, V. Sahore, R. Knob,
A. Nielsen

9:15 – 48. Direct quantification of cancer antigen biomarkers by fluorescent measurement. **H. Li***, S. Ho, D. Xu, R. Wong,
M. Wong

9:35 Break

9:45 – 49. Fabrication of luminescence-based sensor arrays for protein sensing. **X. Zhang***

10:15 – 50. Carbon nanodots as sensitive probes and potential drugs. **H. Chang***

10:35 – 51. Novel fluorescent materials for biochemical applications. **J. Ouyang**

10:55 – 52. Fluorogenic sensors for detection of intracellular reactive oxygen species. **W. Zhong***, Y. Liu, F. Si

11:15 – 53. Ultrasensitive detection of biomolecules using aggregation of functionalized gold nanoparticles. **T. Zako***,
T. Bu, M. Maeda

11:35 Concluding Remarks

Marriott Waikiki Beach
Kona Moku Blrllm B

Symposium on Petroleomics: Molecular Level Understanding of Petroleum for Environmental Science and Petroleum Engineering (#247)

Organized by: S. Kim, Y. Harvey,
A. McKenna

8:00 Introductory remark

8:05 – 54. Introducing petroleomics into molecule-based kinetic models. **M.T. Klein***

8:30 – 55. Characterization, kinetic modeling, and informatics of heavy petroleum fractions. **R. Tanaka***, T. Suzuki,
K. Hagiwara, T. Takada, S. Teratani

8:55 – 56. Application of volcano plots for quantitative visualization and comparison of a set of two spectra obtained by high-resolution mass spectrometric analysis of crude oils. **M. Hur***, S. Kim, R. Beasley,
A.M. McKenna, R.P. Rodgers,
A. Marshall, E.S. Wurtzel

9:20 – 57. Identifying intermolecular interactions in polycyclic aromatic hydrocarbons: DFT calculations and photoacoustic spectroscopy measurements.
F. Spillebout*, K.H. Michaelian,
D. Bégué, J.M. Shaw

9:45 Break

* Principle Author

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10:00 – 58. Sulfur compounds in petroleum: New findings for geochemistry and refining. **Q. Shi***, M. Wang, Y. Zhang, S. Zhao, C. Xu

10:25 – 59. Novel aspect of structural elucidation of petroleum using supercritical fluid chromatography and atmospheric pressure photon-initiated hydrogen/deuterium exchange mass spectrometry. **Y. Cho**, Y. Kim, S. Kim*

10:50 – 60. Joint characterization of asphaltenes and heavy oils using measured and computed infrared and Raman spectra, and enthalpies of solution for molecules and nanoparticles. **J.M. Shaw***

11:15 – 61. New method for determining composition of complex crude mixture. **T. Miao***

Marriott Waikiki Beach
Waikiki Blrm I

Magnetoanalytical Science: Separation, Characterization and Imaging (#320)

Organized by: H. Watarai, I. Fritsch, C. Fuh
Presiding: I. Fritsch, C. Fuh

8:00 Introductory Remarks

8:05 – 62. Prospects of magnetoanalytical science: Application of magnetophoresis and magneto-optical spectrometry. **H. Watarai***

8:30 – 63. Magnetoanalytical analysis using functional nanoparticles. **C. Fuh***, C. Li, S. Yang, J. Chan, Y. Su, H. Tsai

9:05 – 64. Analysis of magneto-optical property change of a single diamagnetic crystal due to the inclination in a microscopic region. **Y. Mizukawa**, M. Iwasaka

9:30 – 65. Developments of *in-situ* optical observation devices utilizable under high magnetic fields. **N. Hirota***, H. Okada, T. Ode, M. Kiyohara, M. Tanokura, A. Nakamura, J. Ohtsuka, H. Wada

9:55 Break

10:10 – 66. Attraction and repulsion – applications of magnetism for bioanalysis in lab on a chip devices. **N. Pamme**

10:45 – 67. Simulation study for material motion induced by magnetic force in fluid. **H. Okada***, N. Hirota, S. Nishijima

11:10 – 68. Magnetic actuation of droplets with or without super paramagnetic particles on superhydrophobic surfaces for digital microfluidic applications. L. Mats, F. Logue, P. Agrawal, **R.D. Oleschuk***

11:35 – 69. Structural change of single-walled carbon nanotubes prepared in magnetic fields. **A. Hamasaki***, J. Uchimura, S. Ozeki, A. SAKAGUCHI, Y. TAKASHIMA

Tuesday Afternoon

Marriott Waikiki Beach
Waikiki Blrm III

New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15)

Organized by: S. Krylov, D. Wilson, W. Zhong, H. Wang
Presiding: H. Wang, D.J. Wilson

13:00 Opening statement

13:05 – 70. Exploring the kinase-substrate interactions by new phosphoproteomics techniques. **H. Zou***, M. Ye, Y. Bian, M. Dong

13:35 – 71. DNA-protein interaction as applied to detection of specific proteins and DNA lesions. **C. Le***, F. Li, Y. Lin, A. Newbigging, R. Palivoda, H. Peng, M. Reid, C. Wang, Z. Wang, X. Yan, H. Zhang

14:05 – 72. Turning electric field induced bacterial aggregation into advantage for the study of interactions between bacteria and macromolecules. N. Sisavath, P. Got, G. Charrière, D. Destoumieux-Garzon, **H. Cottet***

14:25 – 73. Affinity microcolumns as new tools for examining the binding and rates of protein interactions with drugs and hormones. **D.S. Hage***, X. Zheng, S. Beoram, Z. Li, M. Podariu, M. Brooks

14:45 – 74. Partial-filling capillary electrophoresis using lectins and exoglycosidases for profiling glycoprotein glycans. **S. Suzuki**

15:05 Break

15:20 – 75. Analysis of amyloid protein aggregation using microchannel electrophoresis. **C. Hestekin***, S. Paracha

15:40 – 76. Microchip immunoaffinity analysis of a serum biomarker for cancer. **A.T. Woolley***, J.V. Pagaduan, K. O'Neill

16:00 – 77. Determination of acid dissociation constants of phenolphthalein and its derivatives under degradation. **T. Takayanagi***

16:20 – 78. RNA aptamer based assay for thrombin through affinity capture and subsequent enzymatic activity analysis. **Q. Zhao**

16:40 – 79. Single molecule analysis of polysaccharides using a solid state nanopore. **M. Takemasa**, M. Fujita, M. Maeda

Marriott Waikiki Beach
Milo III

Frontiers in Flow Injection Analysis and Related Techniques (#45)

Organized by: T. Imato, G. Christian, K. Grupan, S. Kolev, A. Sabarudin

13:00 – 80. Advances in high speed ion chromatography. **C. Lucy***

13:25 – 81. Over 10 000 peptide identifications from the HeLa proteome using single-shot capillary zone electrophoresis-tandem mass spectrometry. L. Sun, G. Zhu, X. Yan, Y. Zhao, A. Herbert, M. Westphall, M. Rush, M. Champion, J. Coon, **N. Dovichi**

13:50 – 82. Ultrarapid determination of Cr(VI) by stop-flow sequential injection analysis coupled with electrochemical detection using polyaniline-graphene quantum dots-modified screen-printed carbon electrode. **O. Chailapakul**, E. Punrat, C. Maksuk, S. Chuanuwatanakul, W. Wonsawat

14:15 – 83. Advances in chemiluminescence detection for flow analysis. **P.S. Francis***

14:40 Break

14:55 – 84. Flow analyses utilizing periodically varying flow rate: Feedback-based flow ratiometry, and amplitude modulated multiplexed flow analysis. **H. Tanaka***, M. Takeuchi

15:20 – 85. Catalytic flow-injection analysis method using oxidation reaction of *N*-(3-sulfopropyl)-3',5'-tetramethylbenzidine. **M. Kurihara***

15:45 – 86. Specialization of heavy metals in soil sample by sequential extraction used all injection system. **H. Itabashi***, M. Mori, M. Sasaki, H. Shinozaki

16:10 – 87. Monolith: Its applications to flow chemistry. **A. Sabarudin**

Marriott Waikiki Beach
Kona Moku Blrm C

Advances in Analytical Ion Mobility Separations (#61)

Organized by: A. Shvartsburg, F. Misaizu, T. Fukuda

Presiding: F. Misaizu

13:00 – 88. Ion mobility with a focus on field asymmetric waveform ion mobility spectrometry (FAIMS) as an ion filtering tool to aid mass analysis. **S. Prasad***, M.W. Belford, J. Dunyach

13:30 – 89. Differential ion mobility-mass spectrometry for the separation and structure elucidation of isomeric lipids. **S. Blanksby**, A. MacCarrone, T.W. Mitchell

14:00 – 90. Resistively heated temperature programmable gas chromatography with differential mobility spectrometry. M.R. Jacobs, T. Blackstock, R. Gras, J. Luong, **R.A. Shellie***

14:30 – 91. Advances in high-resolution differential ion mobility separations and integration with ETD. **A. Shvartsburg***, A. Bowman, M. Baird, J. Kaszycki, G. Anderson

15:00 Break

15:20 – 92. Multistage differential mobility spectrometry at ambient pressure with ion transformations for enhanced measurement specificity. **G.A. Eiceman**

15:40 – 93. Differential mobility spectrometry for enhanced selectivity in LC-MS analysis of algal biotoxins. **M.A. Quilliam**, E. Kerrin, D. Beach*

16:20 – 94. Combining IMS and OMS techniques with gas-phase HDX-MS/MS measurements for ion structure characterization. **S.J. Valentine***, J. Arndt, M. Khakinejad, S. Ghassabi Kondalaji

Marriott Waikiki Beach
Milo I

Immunoanalysis: Applications and Trends for Environmental Monitoring and Human Health (#94)

Organized by: S. Gee, I. Kennedy, H. Ohkawa, T. Xu, T. Prapamontol

Presiding: I.R. Kennedy

13:00 – 95. Development of an ELISA to detect clenbuterol in pork using a new approach for hapten design. **A.Q. Bui***

13:30 – 96. Principles for design of lateral flow devices for rapid testing for organic and biological chemicals. **I.R. Kennedy***, A.N. Crossan, F. Sanchez-Bayo

14:00 – 97. Immunochromatography: Current advances and trends for agro-product safety. **P. Li, Q. Zhang, z. zhang**

14:30 – 98. New multianalyte lateral flow assays for control of toxic contaminants. **B.B. Dzantiev***, A.V. Zherdev, N.A. Taranova, A.N. Berlinia

14:55 Break

15:10 – 99. Highly sensitive and rapid immunoassay with a novel extraction solution containing a surfactant and a disulfide bond cleaving reagent. **Y. Oyama**, M. Shioji, T. Honjoh

15:40 – 100. Phage-borne anti-immunocomplex peptides and nanopeptides for noncompetitive detection of small analytes. G. Lassabe, A. González-Techera, L. Vanrell, H. Kim, S. Gee, B. Hammock, **G. Gonzalez-Sapienza***

16:05 – 101. One step noncompetitive detection of 3-PBA based on anti-immuno-complex peptide-alkaline phosphatase fusion protein. **J. Dong**, A. González-Techera, S. Gee,

16:30 – 102. Application of new signal probes in immunoassays. **y. zhang***, w. sheng, s. wang

Marriott Waikiki Beach
Kona Moku Blrm A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung

Presiding: Y. Baba, A. van den Berg, T. Yasui

13:00 Introductory Remarks

13:05 – 103. Nano- and quantum-biodevices for cancer diagnosis, cancer therapy, and iPS cell based regenerative medicine. **Y. Baba***

13:30 – 104. Formation of lipid nanoparticles using microfluidic devices. **M. Tokeshi***

13:55 – 105. Real-time detection of biomolecules in live animals. **H.T. Soh***

14:20 – 106. Decoding biological information with quantum chemistry. **M. Taniguchi***

14:45 Break

15:00 – 107. Biomimetic microfabrication for bioanalysis or life science application – lipid vesicles or tubules. **T. Kim***

15:25 – 108. Nanowire devices for analyzing biomolecules. **T. Yanagida**

15:50 – 109. Nanostructures for biomolecule analysis. **T. Yasui***, N. Kaji, T. Yanagida, M. Kanai, S. RAHONG, K. Nagashima, T. Kawai, Y. Baba

16:15 – 110. Integrated microfluidic biochip for label-free isolation of a single cancer cell in blood and for measurement of drug responses on the cell. A. Kamahenehar, T.V. Beischlag, **P.C. Li***

16:30 – 111. Micro- and nanochamber array devices for a single molecule and nucleus analysis. **N. Kaji***, T. Yasui, Y. Baba

16:45 – 112. Development of a single molecular tunnel-current based identification method toward nucleotide sequencing. **T. Ohshiro**, M. Tsutsui, K. Yokota, T. Kawai, M. Taniguchi*

Marriott Waikiki Beach
Milo IV / V

Innovation in Chemical Sensing and Separation Systems toward Advanced Chemical Analysis (#159)

Organized by: T. Hayashita, P. Dasgupta, B. Cho, A. Tong, T. Okada, W. Zhong, H. Li, H. Chang

Presiding: T. Hayashita, W. Zhong

13:00 Introductory Remarks

13:05 – 113. Digital LAMP on a SD chip for point-of-care genetic analysis. **D. Chiu**

13:25 – 114. Surface-bubble-modulated liquid chromatography: A new strategy for manipulating chromatographic retention by pressure-induced change in the volume of stationary nanobubbles.

M. Shibukawa*, K. Nakamura, S. Saito

13:45 – 115. Variation of plasmonic sensor systems for fluid samples. **N. Fukuda***, K. Nomura, M. Fujimaki, H. Ushijima

14:05 – 116. Admittance detection in microsystems: Old wine in a new bottle? **P.K. Dasgupta***, M. Zhang

14:35 – 117. Chirality sensing using coordination polymers of Ag(I) with thiol ligand. Q. Zhang, N. Chen, Z. Li, **Y. Jiang***

14:55 Break

15:05 – 118. Guest-induced supramolecular chirality in ditopic azobis(cyclodextrin complexes in water. **T. Hayashita***, K. Nonaka, M. Yasui, T. Hashimoto

15:25 – 119. Photoresponsive fluorescent molecules in solution and solid state. **A. Tong, Y. Xiang, K. Li, L. Peng**

15:45 – 120. Mitochondrial targeting apoptosis by antitumor theranostic prodrug. R. Kumar, H. Jung, Y. Lee, W. Shin, J. Jang, S. Uhm, K. Sunwoo, W. Kim, S. Koo, **J. Kim***

16:05 – 121. Fluorescence sensors for species of biological and environmental interest. **T.D. James***

16:25 – 122. Sensing of biomedically relevant species in live tissues by two-photon microscopy. **B. Cho***

16:55 Closing Remarks

Marriott Waikiki Beach
Kona Moku Blrm B

Symposium on Petroleomics: Molecular Level Understanding of Petroleum for Environmental Science and Petroleum Engineering (#247)

Organized by: S. Kim, Y. Harvey, A. McKenna

* Principle Author

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2015 program online at:

<http://pacifichem.org/>

onlineprogram

13:00 Introductory Remark
13:05 – 123. Molecular insight into oil spill weathering helps advance high magnetic field FT-ICR mass spectrometry.

A.M. McKenna*, N.K. Kaiser, C.L. Hendrickson, R.P. Rodgers, C.M. Reddy, R.K. Nelson, K. Lemkau, L. Nyadong, D.L. Valentine, Y.E. Corilo, D.C. Podgorski, G.T. Blakney, J.T. Savory, J.P. Quinn

13:30 – 124. True boiling point (TBP) based fractionation of crude oil: Detailed chemical and toxicological characterization.

U. Yim*, S. Ha, A. Loh, W. Shim

13:55 – 125. Closer look at petroleum and the environment using Fourier transform ion cyclotron resonance mass spectrometry.

M.P. Barrow

14:20 – 126. Differentiating natural and anthropogenic sources of bitumen-derived organic compounds to water resources surrounding the Canadian oil sands.

C. Sun*, J. Martin*, . Shotyk, . Poesch, N. Siniatambay

14:45 Break

14:55 – 127. Lignin-derived alicyclic aliphatic structures incorporated into kerogen and petroleum.

P.G. Hatcher, B.E. Hartman,

N. DiDonato, D.C. Waggoner

15:20 – 128. Potential of FTIR for characterizing vacuum distillates.

C. Sanchez*, H. Yarranton, M. Mapolelo, S. Mahavadi,

S. Andersen

15:45 – 129. Seeing is believing - but your petroleum is not what you see!

J.T. Andersson*

16:10 – 130. Understanding solar induced transformation of crude oils using high resolution ion mobility spectrometry coupled to FT-ICR MS.

P. Benigni, K. Sandoval, C.J. Thompson,

M.E. Ridgeway, M.A. Park, P. Gardinali,

F. Fernandez-Lima

16:35 – 131. Supramolecular assembly model for asphaltene aggregation: Mechanistic insights from computational modeling.

S. Stoyanov, A. Kovalevko

Marriott Waikiki Beach
 Waikiki Blrm I

Magnetoanalytical Science: Separation, Characterization and Imaging (#320)

Organized by: H. Watarai, I. Fritsch, C. Fuh
Presiding: H. Watarai, M. Zborowski

13:00 – 132. Magnetic cytosmear for specialized cytological analyses in global health and disease.

M. Zborowski*, L.R. Moore, J.J. Chalmers

13:35 – 133. Chip-scale magnetoresistive platforms for human health diagnostics.

M.D. Porter*, J. Park, C. Lim, J. Beck,

A. Skuratovsky, C. Young, B. Blackley,

G. Khanderao, J. Granger, M. Granger

14:00 – 134. Magnetic particle Imaging: Recent developments and translational applications in cardiovascular disease and molecular imaging of cancer.

K.M. Krishnan

14:35 – 135. Plasmonic-magnetic nanorods for imaging and therapeutics.

J. Chen

15:00 Break

15:15 – 136. Magneto-resonance approaches for antiviral drug designing.

O. Prakash*, D. Takahashi, K. Chang,

Y. Kim

15:40 – 137. Nanoscale magnetometry using the nitrogen-vacancy centre in diamond.

L. Hollenberg

16:15 – 138. Materials and In-fiber devices for magneto cardiology and magneto encephalography applications.

P. Gangopadhyay*

Wednesday Morning

Marriott Waikiki Beach
 Waikiki Blrm III

New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15)

Organized by: S. Krylov, D. Wilson, W. Zhong, H. Wang
Presiding: H. Wang, W. Zhong

8:00 Opening Statement

8:05 – 139. Protein-protein interactions, networks, and structures: New tools for in vivo discovery.

J.E. Bruce*, J.D. Chavez, A. Navare, D. Schweppe, X. Wu, C. Zheng

8:35 – 140. Use of the conditional two-hybrid system to analyse methylation-dependent interactions and protein interaction codes.

M. Wilkins

9:05 – 141. Fluorogenic dyes for screening of protein-nanoparticle interactions.

W. Zhong, J. Ashby, Y. Duari

9:25 – 142. Responsive nanogels for biomolecular separations.

L.A. Holland*

9:45 – 143. Investigation of complex matrix effect on solid phase microextraction for biological sample analysis.

R. Jiang, F. Zhu, G. Ouyang*

10:05 Break

10:20 – 144. Characteristic evaluation of PEG-based hydrogels for protein recognition using molecularly imprinting technique.

T. Kubo, S. Arimura, T. Naito, K. Otuska

10:40 – 145. Generalized model on the effects of nanoparticle on fluorophore fluorescence in solution.

D. Zhang

11:00 – 146. Evaluating the selectivity of functionalized squarylium cyanine dyes towards saccharides and sialic acids.

C.L. Colyer, K. Uchi, T. Maeda,

H. Nakazumi, M. Shibukawa, S. Saito*

11:20 – 147. Covalent peptides to probe protein-protein interactions and modulate signal transduction inside cells.

J. Xia*

11:40 – 148. Ligand/receptor modified hydrogel particles as probes for biomolecular interactions at surfaces.

A. Calaméo, H. Wang, T. Radke, T. Pompe, L. Hartmann, S. Schmidt*

Marriott Waikiki Beach
 Kona Moku Blrm B

Current Issues in Teaching Analytical Chemistry (#38)

Organized by: T. Wenzel, C. Lucy, G. Dicinioski

Presiding: G. Dicinioski, C. Lucy, T. Wenzel

8:00 Introductory Remarks

8:05 – 149. What are the most effective teaching methods for an undergraduate laboratory program?

R. Pullen, G. Dicinioski*, B.F. Yates, N. Brown, J. Smith

8:35 – 150. Incorporating analytical research experience into the undergraduate curriculum.

K. Thurbide

9:05 – 151. Advancing science and engineering through laboratory learning:

ASELL. K.F. Lim

9:35 – 152. Using digital tools to foster active learning.

C.R. Harrison

10:05 Break

10:20 – 153. Free resources for teaching analytical chemistry.

C. Lucy*

10:50 – 154. Two-sided story: Challenges and successes implementing active learning laboratory experiments for an undergraduate analytical chemistry course.

A.G. Cavinato*

11:10 – 155. Use of project-based learning and technology to further engage students in quantitative analysis.

S.C. Russell*

11:30 – 156. Some teaching approaches to stimulate critical thinking in analytical chemistry.

D. Beauchemin

11:50 Concluding Remarks

Marriott Waikiki Beach
 Milo III

Frontiers in Flow Injection Analysis and Related Techniques (#45)

Organized by: T. Imato, G. Christian, K. Grupan, S. Kolev, A. Sabarudin

8:00 – 157. Microfluidic devices for controlling the environment around dorsal root ganglion neurons and collecting stimulated release of transmitters and peptide.

J.V. Swedler*, E.G. Tillmaand, N. Yang, M.A. Makurath, S.S. Rubakhin

8:25 – 158. Membraneless vaporization unit coupled with flow analysis system for determination of volatile compounds.

N. Ratanawarnpong*, T. Pluangklang, W. Al-ahmad, D. Macapricha, P. Wilairat

8:50 – 159. Instrument-free paper microfluidic flow sensors using a mobile phone for potentiostatic control and electrochemiluminescence detection.

C.F. Hogan*

9:15 – 160. Determination of biological samples by flow analysis and its potential to medical support.

N. Teshima*, H. Murakami

9:40 Break

9:55 – 161. Electrodialytic ion-extraction device ion-exclusion chromatography of silicate ion.

M. Mori*, Y. Kurosawa, H. Kojima, N. Nakatani, S. Ohira, K. Tsunoda, H. Itabashi

10:20 – 162. Flow injection analysis of β -secretase activity by using of immobilized recombinant fusion β -secretase and application of the system for the inhibitor.

Y. Iida*

10:45 – 163. Flow immunoassay based on carbon nanodots.

R. Ishimatsu, K. Nakano, T. Imato

11:05 – 164. Specific fluid behavior of the mixed solutions in a micro-space and its application.

S. Fujinaga, M. Hashimoto, K. Tsukagoshi, J. Mizushima

Marriott Waikiki Beach
 Kona Moku Blrm C

Advances in Analytical Ion Mobility Separations (#61)

Organized by: A. Shvartsburg, F. Misaizu, T. Pukala

Presiding: A. Shvartsburg

8:00 – 165. Analysis of the three-dimensional shape of polyatomic ions by ion mobility spectrometry.

T. Wyttenbach, C. Bleiholder, M.I. Bowers*

8:30 – 166. Structural characterisation of biomolecular assemblies by chemical cross-linking and ion mobility-mass spectrometry.

M. Graetz, A. Button, T.L. Pukala*

9:00 – 167. Integrated ion mobility and mass spectrometry methods for structural proteomics.

B. Ruotolo*

9:30 – 168. Probing structural dynamics and aggregation of human islet amyloid polypeptide using Ion Mobility Mass Spectrometry.

H.I. Kim*, S.C. Lee, S. Akashi, M. Lim

10:00 Break

10:20 – 169. Understanding biopolymer structures and folding in solution from studies of naked ions in the gas phase.

D.E. Clemmer*

10:50 – 170. Intact membrane proteins released from detergent micelles under vacuum: Combining IMS/MS, in silico collision-induced dissociation and molecular dynamics simulations.

F. Montenegro, M. Barrera, S. Torres, N.P. Barrera*

11:20 – 171. HDX-TIMS-MS reveals kinetic intermediates of globin proteins.

C. Harrilal, J. Molano-Arevalo,

E.R. Schenk, J. Miksovská,

F. Fernandez-Lima

Marriott Waikiki Beach
 Milo I

Immunoanalysis: Applications and Trends for Environmental Monitoring and Human Health (#94)

Organized by: S. Gee, I. Kennedy, H. Ohkawa, T. Xu, T. Prapamontol

Presiding: T. Xu

8:00 – 172. Single domain heavy chain antibodies (nanobodies or VH): Monoclonal antibody replacement?.

B. Hammock*, S. Gee

8:25 – 173. Environmental and human exposure monitoring for tetrabromobisphenol A by immunoassays based on a variable domain of heavy chain antibody.

T. Xu*, J. Wang*, C. Bever*, S. Gee*, Q.X. Li, B. Hammock

8:50 – 174. Synthetic biology immunosensors: Whole-cell biosensors based on surface displayed nanobodies.

K.M. Polizzi*, H. Lai, N. Kyllilis, P.S. Freeman

9:10 – 175. Nanobody based ELISA for protein and small molecule detection using a polymeric enzyme as the label.

D. Li, Y. Cui, S. Gee, Y. Ying, B. Hammock

9:30 – 176. Single domain antibodies to haptens: Selection strategy and unusual binding properties.

S. Tabares, M. Pirez, L. Wogulis, D. Wilson, B.M. Brenna, G. Gonzalez-Sapienza*

9:50 Break

10:05 – 177. Camelid derived VHJs as new generation immunoanalysis reagent for environmental chemicals - aflatoxin as an example.

A. Wei*, J. Herron, X. Wang, A. Zinkl

10:30 – 178. Development of visual screening examination kit for cadmium by immunochromatography using anti-(Cd-EDTA) antibody.

H. Arai*, K. NAKAMURA, Y. YOSHIDA,

K. TAWARADA

10:55 – 179. ELISA coupled with solid phase microextraction on a modified polysiloxane waveguide.

G. Mackey, K. Flynn, R. Brown*

11:15 – 180. Detection of the tuberculosis antigenic marker lipoarabinomannan in infected patient sera by gold nanoparticle labeling and surface-enhanced Raman scattering.

M.D. Porter*, A. Crawford, L. Laurentius, T.S. Mulvihill, J. Granger, J. Spencer, D. Chatterjee, K. Hanson

11:35 – 181. Detection of β -agonists by noble metal nano-materials based surface-enhanced Raman scattering immuno-chromatographic assay.

A. Deng

Marriott Waikiki Beach
 Kona Moku Blrm A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung

Presiding: J. Ramsey, S.A. Soper, D. Spence

8:00 Introductory Remarks

* Principle Author

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- 8:05 – 182.** Rapid electronic identification of individual molecules with single nanometer-scale pores. **J. Kasielowicz***, A. Balijepalli, J. Benjamini, J. Robertson, H. Wang, J. Forstater, J. Reiner
8:30 – 183. Interfacing nanofluidic devices to the real world: Analyzing drug-induced damage in single DNA molecules isolated from circulating tumor cells. **S.A. Soper***
8:55 – 184. Nanofluidic devices for the manipulation and characterization of DNA: One molecule at a time. L.D. Menard, O.A. McCrate, M.A. Tycon, **J. Ramsey***
9:20 – 185. Microengineering intestine for biomedical assays. **N. Albritton**
9:45 Break
10:00 – 186. Biomimetic channels and channel networks. **A. Manz**
10:25 – 187. Enhanced, rugged organ-on-chip systems with 3D-printed devices. **D. Spence**
10:50 – 188. Compact microfluidic systems for low-cost chemical and biological analyses. **C.J. Backhouse***
11:15 – 189. Nanomechanical devices as a molecular sensing platform. T. Biswas, N. Miriyala, T. Thundat, K. Beach, **J.P. Davis***
11:30 – 190. Development of microfluidic plasma separation device for whole blood immunoassay. **H. Shimizu**, M. Kumagai, E. Mori, K. Kawatari, T. Kitamori*
11:45 – 191. Bioinspired conducting polymers to couple cells electrically at high selectivity. Q. Pan, Y. Zhang, **B. Zhu***, Y. He

Hawaii Convention Center
Halls I, II, III

Innovation in Chemical Sensing and Separation Systems toward Advanced Chemical Analysis (#159)

Organized by: T. Hayashita, P. Dasgupta, B. Cho, A. Tong, T. Okada, W. Zhong, H. Li, H. Chang
Presiding: T. Hayashita, W. Zhong

Poster Session

10:00 – 12:00

- 192.** siRNA separation and identification by capillary polymer electrophoresis. C. Liu, Y. Yamaguchi*, **X. Dou**
193. Development of temperature-responsive solid-phase extraction column for biological sample pretreatment. **M. Akimaru***, K. Okubo, Y. Hiruta, H. Kanazawa
194. Effects of terminal group and chain length on temperature-responsive chromatography utilizing Poly(*N*-isopropylacrylamide) via RAFT polymerization. **Y. Nagumo***, Y. Hiruta, H. Kanazawa
195. Application of quinoline oligoamide folamer for chiral HPLC stationary phase. **H. Noguchi**, V. Maurizot, M. Takafuji*, I. Huc, H. Hara*
196. Ice grain boundary as a size-selective electrophoretic separation field. **A. Inagawa**, T. Okada
197. Shear flow ice chromatography. **M. Shimizu**, M. Harada, T. Okada
198. Chiral separation with composite-type stationary phase. **Y. Ilimura**, T. Okada
199. Designing novel potentiometric sensors based on nanostructured TiO₂ electrodes for selective determination of biologically important transition metals in real samples. **M. Hariri***, S. Morin
200. Adsorption behavior of Cu(II)-ammonia complex to gel-like solid polyol compounds through dehydration condensation reaction. **T. Fujimori***, H. Mabuchi, K. Yoshimura
201. Efficient recovery of rare metals ions with calix[4]arene derivatives by using droplet-based microreactor system in nitric acid media. R. Sathuluri, M. Maeki, K. Ohto, **M. Miyazaki**
202. New approach toward fast and efficient DNA aptamer selection for microbial cells using polymer-enhanced capillary transient isotachophoresis. **K. Hirose***, M. Tsuchida, K. Yoshimoto, C.L. Colyer, M. Shibukawa, S. Saito

- 203.** Evaluation of the intrinsic retention selectivity of hydrocarbonaceous and fluorocarbonaceous stationary phases by surface-bubble-modulated liquid chromatography. **K. Nakamura***, S. Saito, M. Shibukawa
204. Development of an off/on fluorescence probe for carbonic anhydrase IX based on twisted intramolecular charge transfer (TICT) state. **S. Takahashi***, K. Hanaoka, Y. Urano
205. Recognition and optical sensing of phenylurea pesticides by carboxylate anion. **R. Kato***, H. Okumura, K. Ito, T. Hattori
206. Preparation and characterization of anion sensing polymer nanofibers and its anion sensing properties in methanol and methanol-water. **H. Kahara***, R. Kato, T. Hattori, Y. Ishii
207. Visual measurement of contaminants using a thiokolptic gel. **T. Saito***
208. Laser trapping induced microparticle formation in thermoresponsive polymer/alcohol/water ternary system and its application for ultratrace analysis. **R. Nohara**, A. Miura, N. Kitamura
209. Recognition function of phosphate derivatives by supramolecular dipicolyl-amino azoprobe/dendrimer complexes in water. **T. Hashimoto**, A. Koshino, Y. Tsuchido, T. Hayashita*
210. Development of fluorescent probe possessing dipicolylamine for selective ion recognition in water. **Y. Torii**, M. SAWADA, S. Fujiwara, T. Hashimoto, T. Hayashita*
211. Design and function of dipicolylamine fluorescent probes for ion recognition in water. **M. SAWADA**, Y. Torii, H. KOBAYASHI, T. Hashimoto, T. Hayashita*
212. Substituent effect on recognition of phosphate derivatives by dipicolylamine azoprobe/cyclodextrin complex sensor. **S. MINAGAWA**, T. UEMURA, T. Hashimoto, T. Hayashita*
213. Long-time nonadiabatic molecular dynamics of boronic acid fluorophore. **O. Kobayashi***, S. Narbu
214. Development of supramolecular rotaxane sensors possessing ion recognition function by biscrown ether structure. **M. OKANIWA**, S. MURAYAMA, S. Fujiwara, Y. Tsuchido, T. Hashimoto, T. Hayashita*
215. Evaluation of sugar adsorption gel based on phenylboronic acid azoprobe/cyclodextrin complexes. **T.G. Bekele**, T. Yamada, T. Suzuki, T. Hashimoto, T. Hayashita*
216. Design of saccharide recognition material based on boronic acid fluorophore/cyclodextrin supramolecular complex. **T. Suzuki**, Y. Tsuchido, T. Hashimoto, T. Hayashita*
217. Selective sugar recognition by fluorinated boronic acids fluorophore/cyclodextrin complexes in water at neutral pH condition. **K. Sugita**, Y. Tsuchido, T. Hashimoto, T. Hayashita*
218. Saccharide recognition by using amphiphilic phenylboronic acid sensor. **Y. Tsuchido**, T. Suzuki, R. Sato, T. Hashimoto, T. Hayashita*
219. Design and function of dipicolylamine modified β -cyclodextrin for phosphate anion sensing in water. **S. Fujiwara**, T. Yamada, H. KOBAYASHI, T. Hashimoto, T. Hayashita*
220. Design and function of supramolecular dipicolylamine-modified cyclodextrins. **T. Yamada**, S. Fujiwara, H. KOBAYASHI, T. Hashimoto, T. Hayashita*
221. Development of bacteria detection sensor based on phenylboronic acid/dendrimer complex supramolecular in water. **R. Horiuchi**, Y. Tsuchido, H. KOBAYASHI, T. Hashimoto, T. Hayashita*
222. Development of fluorescent probe for pathogenic bacterial detection. **Y. Kasai**, H. KOBAYASHI, Y. Tsuchido, T. Hashimoto, T. Hayashita*
223. Novel electrochemical molecular recognition system using metal complexes assembled on gold nanoparticles. **A. Endo***, S. Yoshimoto, T. Hashimoto, T. Hayashita
- 224.** Electrochemical molecular recognition of the dopamine with the ruthenium complexes assembled on metal nanoparticles. **A. Sunata**, A. Endo, T. Hashimoto, T. Hayashita*
225. Molecular recognition using a β -cyclodextrin assembled on the gold electrode by impedance spectroscopy (EIS). **N. Ishiguro**, T. Hashimoto, A. Endo, T. Hayashita

- Marriott Waikiki Beach
Waikiki Blrm I
- Magnetoanalytical Science: Separation, Characterization and Imaging (#320)**
- Organized by:* H. Watarai, I. Fritsch, C. Fuhr
Presiding: I. Fritsch, N. Pamme
- 8:00 – 239.** Expanding lab-on-a-chip applications for redox-magnetohydrodynamic microfluidics through polymer-modified electrodes and enhanced current-magnet relationships. **F.Z. Khan**, B.J. Jones, K.C. Nash, **I. Fritsch***
8:35 – 240. Electrochemical detection of magnetic field-induced agglomeration of solution-phase Fe₃O₄ nanoparticles. **K. Tschulik***, R.G. Compton
9:00 – 241. Magnetic enrichment for ultra-trace electrochemical detection of chiral Pt-decorated iron oxide nanoparticles. **K.J. Stevenson***, D. Robinson
9:25 – 242. Effects of magnetic field and metal nanoparticles on photoelectrochemical reactions of porphyrin-viologen linked compound-metal nanoparticle composite films. **H. Yonemura***, T. Niimi, S. Yamada
9:50 Break
10:05 – 243. Chiral surface formation by galvanostatic magnetoelectrodeposition. **I. Mogi***, R. Aogaki, K. Watanabe
10:30 – 244. Tailored magnetic fields for controlling the electrochemical deposition of metal. **G. Mutschke***, S. Mühlhöfer, X. Yang, K. Eckert, K. Tschulik, M. Uhlemann, J. Froehlich, A. Bund
10:55 – 245. FT-IR spectroscopic study on a magnetically treated aqueous solutions using principal component analysis. **K. Suzuki**, T. Hasegawa*, **F. Kimura**, T. Shimoaka, T. Kimura*
11:20 – 246. Development of Faraday rotation imaging microscope with pulsed magnetic field. **M. Suwa**, S. Tsukahara, H. Watarai
- 11:45 Closing Remarks**
- Hawaii Convention Center
Halls I, II, III
- Symposium on Petroleumomics: Molecular Level Understanding of Petroleum for Environmental Science and Petroleum Engineering (#247)**
- Organized by:* S. Kim, Y. Harvey, A. McKenna
- Poster Session**
- 10:00 – 12:00
- 232.** Quantitative observation of change in ring type distribution of UV and natural degraded oil samples. **D. Kim**, S. Ha, U. Yim, W. Shim, S. Kim*
233. Application of molecular dynamic simulation for theoretical collisional cross-section calculations of long-chain alkyl aromatic compounds. **D. Lim**, A. AHMED, S. Kim*
234. Combining chromatographic fractionation and FT-ICR MS analyses for more detailed molecular level identification of crude oil compounds. **J. Ha**, D. Kim, S. Kim*
235. Source characterisation of polycyclic aromatic hydrocarbons (PAHs) in sediments and soils from Khuzestan province, Iran, using multivariate data analysis (CHEMSIC - chemometric analysis of selected ion chromatograms). **J.S. Lübeck**, K.G. Poulsen, S.B. Knudsen, M. Soleimani, J.H. Christensen
236. Characteristic curvature evaluation of anionic surfactants for enhanced oil recovery applications. **A.B. Mejia***
237. Suppression of tar emission by enhancing volatile-char interaction during coal gasification at low temperature. **Y. Kawabata**, T. Wajima, H. Nakagome, S. Hosokai, Y. Suzuki, H. Sato, K. Matsuo
238. Phenol-selective mass spectrometric analysis of petroleum fractions. **H. Zhu***, J. McIndoe

* Principle Author

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- 250.** Development of fluorescence probe for cellular imaging utilizing a temperature-responsive polymer. **A. Yamada***, J. Wang, Y. Hiruta, H. Kanazawa
- 251.** Hollow polymer nanocapsules - new platform for application as optical sensors. **M. Kim**, S. Dergunov, E. Lindner, E. Pinkhasik
- 252.** Label-free cancer cell detection using conducting polymer film. **K. Numada**, H. Shigi, T. Nagaoaka, I. Nakase, S. Tokonami*
- 253.** Design of bright fluorescent polymers for bioassays. **Y. Takahashi**, T. Toyama, R. Kato, Y. Hiruta, Y. Shindo, K. Oka, M. Takai, N. Iwasawa, D. Citterio, K. Suzuki*
- 254.** Colorimetric analysis of chirality using poly(phenylacetylene) with chiral amide receptors. **Y. Moto***, S. Umeda, K. Tsuda, T. Sato, T. Kakuchi, R. Sakai
- 255.** Chiral discrimination of optically active carboxylic acids using polydiacetylene with chiral amino groups at the side chain. **R. Sakai***, Y. Moto, S. Umeda, K. Tsuda, T. Sato, T. Kakuchi
- 256.** Ratiometric detection of protein kinase activity with a fluorescent polyion complex nanoparticle that incorporates an internal standard. **T. Nobori***, S. Shiosaki, A. Kishimura, T. Mori, Y. Katayama
- 257.** Plasmonic full color sensor by use of multilayered metallic nanoparticle sheets. S. Shinohara, D. Tanaka, K. Okamoto, **K. TAMADA***
- 258.** Colorimetric DNA detection by invasive reaction coupled with nicking endonuclease-assisted nanoparticles amplification. **B. Zou**
- 259.** Fluorescent core-shell-type labeling nanoparticles for immunoassays. **K. Osada**, Y. Katayama, K. Suzuki, D. Citterio*
- 260.** Sensing microbes using Au substrates modified with artificial siderophore- Fe^{3+} complexes. **T. Inomata***, H. Ido, T. Murase, T. Ozawa, H. Masuda
- 261.** Determination of cholera toxin based on β -galactose derivative functionalized Au surface. **D.T. Jeong***, K. Ahn, W. Lee
- 262.** Highly sensitive and stable biosensing probes based on Ag containing nanoheterostructures. **A.T. Dao***, D.M. Mott, S. Maenosono
- 263.** Bioluminescent sensing of toxic substance in environmental water by using luminous *Escherichia coli*. **H. Karatani***, D. Okamoto, Y. Ihara
- 264.** Synthetic coelenterazine derivatives for bioluminescence applications. **R. Nishihara**, S. Kim, T. Nakajima, M. Sato, S. Nishiyama, N. Iwasawa, D. Citterio, K. Suzuki*
- 265.** Electrogenenerated chemiluminescent sensor for hydrogen peroxide based on a cyclometalated $\text{Ir}(\text{III})$ complex. **I. Shin**, H. Kim, J. Hong
- 266.** Electrogenenerated chemiluminescence sensor based on sol-gel incorporated CdSe/ZnS quantum dot. **S. Nam***, W. Lee
- 267.** Design of bright chemiluminescent dyes for bioanalysis. **M. Sumiya***, M. Iwama, M. Yokoo, S. Nishiyama, D. Citterio, K. Suzuki*
- 268.** Design and synthesis of novel coelenterazine derivatives with high functionality. **M. Abe**, R. Nishihara, T. Nakajima, M. Sato, S. Kim, N. Iwasawa, D. Citterio, S. Nishiyama, K. Suzuki*
- 269.** Design and synthesis of novel red-shifted firefly luciferin analogs. **Y. Ikeda**, T. Toyama, Y. Adachi, N. Iwasawa, D. Citterio, S. Nishiyama, K. Suzuki*
- 270.** Metal ion-zeolite composite gas sensors for the selective detection of hydrocarbons. **D.C. Pugh***, S.M. Hailes, I.P. Parkin
- 271.** Fiber-optic biochemical acetone gas sensor (bio-sniffer) for assessment of lipid metabolism from exhaled breath. **M. Ye**, P. Chien, K. Toma, T. Arakawa, K. Mitsubayashi*
- 272.** Fiber-optic biosensor with a UV-LED excitation system for sensitive determination of sorbitol-induced diabetic complications. **T. Gessie**, Y. Takimoto, A. Monkawa, T. Arakawa, K. Mitsubayashi*
- 273.** Trace water determination by means of fiber optic gas sensor with metal organic framework as a sensing material. **S. Ohira**, Y. Miki, M. Endo, N. Nakamura, Y. Hirose, K. Toda
- 274.** Highly sensitive and rapid gas biosensor for formaldehyde. **Y. Takimoto**, T. Gessie, N. Jo, A. Monkawa*, T. Wada, N. Sanari
- 275.** Atomically precise doping interrupted chalcogenide-based semiconductor zeolitic analog with tunable photo-/electrochemical property. **Y. Liu**
- 276.** Detection of heavy metal ions and phosphates using organic field effect transistors functionalized with dipicolylamine derivatives. **T. Minami***, T. Minamiki, Y. Sasaki, S. Tokito
- 277.** Development of biocompatible ion sensors based on sol-gel glass modified chemically with oligoethylene glycol derivative. **H. Ishigaki***, S. Yajima, M. Tanaka, K. Kimura
- 278.** Colorimetric cheletating reagents for serum iron and copper based on charged quinone structures. **R. Endo**, Y. Kaneko, K. Kina, N. Iwasawa, S. Nishiyama, D. Citterio, K. Suzuki*
- 279.** On-chip DNA methylation analysis by a bulge specific immuno-recognition. **R. Kurita***, H. Yanagisawa, K. Yoshioka, O. Niwa
- 280.** Multiplexed profiling of cell surface glycans in MALDI-MS by DNA labeling and signal amplification. **Z. He***, J. Lin
- 281.** Observation of conformational changes of a functional RNA by using a quartz crystal microbalance with energy dissipation technique. **H. Furusawa**
- 282.** Characterization of the DNA aptamer which binds to CD4 and its application for detection of CD4-expressing cells. **K. Yano***, T. Shibata, Y. Sato, H. Kubo, T. Shimizu, A. Shiratani, M. Shimizu, A. Sato
- 283.** Toward DNA-detecting FET devices with ligand-immobilized gate surface. **A. Michikawa**, R.K. Verma, N.B. SABANI, K. NAKATANI
- 284.** PEP-on-DEP: A real-time biosensor chip for unreachable biomarker-based diagnostics. **M. Biyani***, K. Kawai, M. Chikae, M. Biyani, H. Ushijima, K. Kitamura, T. Yoneda, Y. Takamura
- 285.** 2D ATP imaging based on CCD type pH sensor modified with ATPase. **S. Endo**, A. Kono, R. Kato, K. Sawada, T. Hattori*
- 286.** 2-Propanol fluorometric biosensor based on secondary-alcohol dehydrogenase (S-ADH) for clinical diagnosis of ketoacidosis. **P. Chien**, M. Ye, K. Toma, T. Arakawa, K. Mitsubayashi*
- 287.** Circularly permuted fluorescent protein-based indicators for citrate. **Y. Honda**, K. Kirimura
- 288.** Visualization of toxic substance in environmental water by using blue fluorescent *Escherichia coli*. **Y. Ihara**, D. Okamoto, H. Karatani*
- 289.** Bioinspired post-polymerization modifications of molecularly imprinted protein recognition nanocavity for acquiring signal transducing function of binding events into fluorescence change. **H. Sunayama**, T. Takeuchi
- 290.** Detection of protein kinase activity using chemical and electrochemical sensors. I. Shin, S. Lee, H. Rhee, **J. Hong***
- 291.** LSI-based microelectrode array chip device with 400 addressable sensors toward electrochemical imaging of stem cells. **Y. Kanno**, K. Ino*, C. SAKAMOTO, K. INOUE Y., M. MATSUDAIRA, A. SUDA, R. KUNIKATA, H. Abe, H. Shiku, T. Matsue*
- 292.** Evaluation of plasticized potentiometric membranes for ion-selective electrodes by pulsed NMR analyses. **T. Moriuchi***, Y. Urabaha
- 293.** Electrodeposition of copper oxide/poly-pyrrole/reduced graphene oxide as a nonenzymatic glucose biosensor. **P. Woi***, P.M. Nia, Y. Alias
- 294.** Oxygen-dependent behavior of the amperometric signals of glucose oxidase enzyme electrodes. **N. Halder***
- 295.** Electrochemical immunochromatography integrated with microperiodic array-based sensor for bioanalyses. **W. Iwasaki***, R. Sathuluri, O. Niwa, M. Miyazaki
- 296.** Novel nanofiber web-based dry electrodes for long-term biopotential monitoring. **L. Jin**, Y. Ahn, K. Kim*, T. Oh, E. Woo
- 297.** Selective nitrogen doped carbon thin film electrode for electrochemical biosensor. **T. Kamata**, D. Kato, O. Niwa*
- 298.** Design of polyion complex sensor arrays that fingerprint secretomic signatures of cells for markerless and noninvasive cell evaluation. **S. Tomita***, K. Yoshimoto, R. Kurita, O. Niwa
- 299.** Non-invasive mouth guard biosensor for continuous measurement of saliva glucose. **T. Arakawa**, Y. Kuroki, H. Nitta, S. Takeuchi, T. Sekita, S. Mizukuchi, K. Mitsubayashi*
- 300.** Interdigital capacitors for monitoring the quality of ethanol lended gasoline using imprinted titania coatings. **A. Mujahid**, M. Irshad, W.u. Zaman, T. Hussain, A. Afzal, N. Iqbal
- 301.** Direct imaging of acetylcholine with a novel fMRI nanosensor. **Y. Luo***, H.A. Clark
- 302.** Development of a high-contrast fluorescence microscopy based on polarization techniques using an optical interference mirror slide. **M. Yasuda***, T. Akimoto
- 303.** Novel "dead volume-free" spotter aspirating and dispensing nanoliter-level samples and its applications to bioanalysis. **H. Aoki**
- 304.** Detection of biomarkers via aptamer based binding events. **M.F. Ali***, S. Situla, J. Grennell, C. Dunlock

Hawaii Convention Center

Halls I, II, III

Analytical General Posters

10:00 – 12:00

Theory and Fundamental Science

324. New viewpoint of potential-dependent component of EDL. **X. Zhao***, J. Chen, Z. Sha, X. Wang, N. Tang**325.** Kinetics of diffusion-limited sorption in the mesoporous silica gel/water system by single microparticle injection and confocal fluorescence microscopy. **T. Sato**, K. Nakatani**326.** Kinetic analysis of chelate extraction at water microdroplet/oil interface by microelectrochemistry and confocal fluorescence microscopy. **N. Sawada**, T. Sato, K. Nakatani***327.** Syntheses and properties of iridium(III) complexes with boronic acid ligands and their reactivity towards D-fructose. **M. Takata***, T. Sugaya, K. Ishihara**328.** Relative kinetic reactivities of boronic acid and boronate ion. **Y. Suzuki**, D. Matsukawa, T. Sugaya, K. Ishihara*

Analysis of Material Structure and Properties

329. Application of the superhydrophobic biomimetic chip in SERS analysis. **Z. Yu***, Y. Jung*, Q. Cong***330.** Water state and gelling process of methyl cellulose thermo reversible hydrogels containing polyethylene glycol and salt. **H. Eguchi***, E. SHIMODA, T. SUZUKI, Y. Nishimoto**331.** Characterization and drying property of lacquer lacquer. **R. Lu****332.** Liquid-liquid phase transition of hydroxylamine-doped water confined within MCM-41 pores, observed by DSC and Raman spectroscopic measurements. **S. Yoshidome***, Y. Ito, A. Nagoe, T. Sugimoto, H. Fujimori**333.** Adsorption behavior of metal ions onto modified mesoporous silicate MCM-41 having Schiff base structure. **S. Oshima**, Y. Watanabe, K. Fujinaga, G. Stevens, Y. Komatsu**334.** Phase transition behavior of acetonitrile – water mixture confined in mesopores. **M. Nakada**, T. Takashi, H. Yoshida

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- 335.** Effect of composite material on deposition behavior of electroless Ni plating. **T. Suzuki***, R. Suzuki, K. Noda
- 336.** Study of SEI layer formed on graphite anodes in a lithium ion battery using NMR, XPS, and FTIR spectroscopy. **S. Jung***, S. Kang
- Analytical Techniques and Methods**
- 337.** Electrocapillary curves at the polarized nitrobenzene/electrolyzed alkaline water interface. **K. Arai***, M. Okajima, M. Ikeda
- 338.** Physicochemical properties prediction of atmospheric distillates (199–371°C+) from its raw crude oils by FTIR-ATR and multivariate analysis. **B. Murciano**
- 339.** Development of rapid direct analysis method for plasticizers in polyvinyl chloride (PVC) product using direct analysis in real time–orbitrap mass spectrometry (DART–OTMS). **Y. Abe***, M. Yamaguchi, M. Mutsga, H. Akiyama
- 340.** Development of flow-balanced ICP torch for low gas consumption and oxide decrease. **N. Yarie***, H. Inoue, K. Kakegawa, H. Miyahara, A. Okino
- 341.** Development of sample collected method using a pyrolyzer. **R. Ozaki**, T. Honda
- 342.** Amperometric zirconia-based sensor attached with NiFe₂O₄ sensing-electrode for selective NO₂ detection. **S. Yoshida**, H. Ikeda, S.A. Anggraini, N. MIURA*
- 343.** Potentiometric YSZ-based gas sensor by using graphite as a novel sensing-electrode. **T. Fujii**, H. Ikeda, S.A. Anggraini, N. MIURA*
- 344.** Evaluation of electropolymerized poly(o-phenylenediamine)-coated micro-electrode arrays for oxygen sensing applications. **M. Patrick***, D. Paul
- 345.** X-ray fluorescence rapid analysis by fusion bead method for materials on Ni extraction process. **S. Kim***, S. Jung, S. Kim
- 346.** Development of an absolute quantification method for food additives in processed foods by ¹H quantitative NMR. **T. Ohtsuki***, K. Sato, Y. Abe, A. Tada, N. Sugimoto, H. Akiyama
- 347.** ²⁷Al NMR quantitative analysis of hydrolysis equilibria for solution containing aluminum polynuclear complex. **G. Sakata**, H. Maki, M. Mizuhata
- 348.** AQAR vs. PULCON: A comparison of qNMR: Internal and external reference methods. **N. Sugimoto***, M. Takada, K. Ishizuki, T. Ohtsuki, A. Tada, Y. Nishizaki, T. Suematsu, T. Miura, Y. Yamada, T. Horinouchi, R. Koike, T. Kato, T. Togawa, H. Akiyama
- 349.** Development of visual analysis of fluoride using test paper with On-OFF color change reaction. **S. Fukuiage**, A. Manaka*, M. Tatu, M. Irie, S. Igarashi
- 350.** Use of a rotating disc electrode with ferricyanide to detect deficiencies in swollen nafion membranes. **M.K. Reynolds***, D. Paul
- 351.** Immobilization of glucosamylase on cellulose supports by covalent binding for increased saccharification stability. **T. Sakamoto**, R. Harada, M. Sakata*
- 352.** Analysis of electrode reactions in a coulometric flow cell for on-line redox derivation liquid chromatography. **K. Saitoh***, H. Tsujimoto, H. Asamoto, M. Shibukawa, T. Nakagama
- 353.** Development of photothermal heterodyne-interferometric detection method as micro-HPLC detector. **M. Isoda**, M. Fukuma, A. Harata*
- 354.** Role of diffusion in band broadening of large particles in capillary electrophoresis. **A. Khodabandehloo***, D.D. Chen
- 355.** Condensed phase membrane introduction mass spectrometry - direct electron ionization (CP-MIMS-DEI): A novel approach for the direct, on-line measurement of PAHs in aqueous samples. V. Termopoli, G. Vandergrift, L. Magrini, G. Famiglini, P. Palma, E.T. Krogh, A. Cappiello, **C.G. Gill**
- 356.** Recent advances of LIBS diagnosis for plasma facing materials in fusion devices. **H. Ding***

Environmental, Forensic and Toxicological Analysis

- 357.** Development of new microanalytical method by Gecko Tape: Analysis of lacquer film. **Y. Nagai**, Y. Kamiya, T. Honda
- 358.** Comprehensive analysis using THM-GC/MS of excavated relics at the Jomon period. **A. Watanabe**, T. Honda
- 359.** Speciation of metal complexes with biodegradable chelants in solution by LC-QTOF-MS. **M. Takemura**, H. Sawai, I.M. Rahman, K. Kudo, T. Maki, H. Hasegawa
- 360.** Investigations of the influence of cations on humic acid and biomembrane interaction. **R. Williams***, H. Olivier, R.L. Cook
- 361.** VOC-adsorption and desorption properties of charcoal prepared from woody biomass. **N. Inomata***, T. TSUGOSHI, T. OKABE, Y. Nishimoto
- 362.** Non-targeted screening and mapping the distribution of organo-brominated compounds in sediments of Lake Michigan. **h. peng***, c. chen, J. Sun, D. Saunders, G.P. Codling, M. Hecker, S. Wiseman, P.D. Jones, J. Giese
- 363.** Analytical study of excavated and natural whetstone at the Owari Domian Upper Mansion site. **Y. Aoyanagi***, M. TAKAOKA, Y. Nishimoto
- 364.** New method for determining styrene oligomers from debris polystyrene and how they contribute to ocean contamination. **K. Koizumi***, H. Sato, H. Katsura, B. Kwon, S. Chung, N. Maximenko, K. Takatama, K. Saito
- 365.** Diversity analysis of trace elements in precious coral using μ -XRF. **K. Kudo***, H. Sawai, T. Maki, Y. Tamenori, T. Yoshimura, N. Iwasaki, H. Hasegawa
- 366.** Behavior of phosphate adsorption on zirconium-loaded activated carbon, and its application for phosphate recovery from seawater. **T. Wajima***
- 367.** Localization of radioactive and nonradioactive cesium in brown rice grains contaminated by fallout from the Fukushima Daiichi Nuclear Power Plant accident. **M. Kato**, Y. Okada, S. Hirai, S. Saito, M. Shibukawa*
- 368.** Use of fermented bark as a soil amendment for cadmium and cesium uptakes in rice. **S. Kobayashi***, M. Mori, T. Ito, H. Itabashi, K. Hatano
- 369.** Harmful-reagent-free separation and concentration system of minor or trace element using melting of a eutectic. **Y. Nishimoto***, T. Takei, R. SUZUKI
- 370.** Determination of trace cadmium in environmental samples by flame atomic absorption spectrometry with preconcentration using sodium dodecyl sulfate/activated carbon. **M. Furukawa**, S. Kaneko*, H. Katsumata, T. Suzuki
- 371.** Development of a DNA-based biosensor for rapid detection of *Reinibacterium salmoninarum*. **T.N. Keohokalole-Look***, A.M. Olivo, B. Mandella, A.G. Cavinato
- 372.** Sampling method for p-nitrophenol in diesel exhaust emissions from actual vehicles meeting the newest regulation. **K. KOSHIKI***
- 373.** Effect of salt stress on the accumulation level of mineral and vitamin C in *Ulva pertusa*. **A. Yamamoto***, M. Moriyama, M. Kurotani
- 374.** Adsorption properties of banana fiber to metal ions. **T. Kajiyama***, K. Arai, H. Kukusen
- 375.** Examination of quantification methods of quercetin in food additives and re-agents using ¹H quantitative NMR. **A. Tada***, N. Sugimoto, Y. Nishizaki, S. Matsuda, H. Kawasaki, K. Ishizuki, T. Ohtsuki, M. Tahara, T. Suematsu, Y. Yamada, H. Akiyama
- 376.** Effects of preparation techniques on availability of health-promoting components and properties of carrots and blueberries. **L. Yu**, B. Gao, L. Yu*
- 377.** Method development and validation for furan analysis in eight different types of food matrices using SPME-GC/MS. **S. Jeong**, Y. SEOK, h. Song, J. Her, K. Lee
- 378.** Quick determination of migration of bisphenol A by an on-line disk and HPLC. **Y. Wang***, X. Chen*, Y. Jiang*, H. Kang*, F. Luo*
- 379.** Ultrasensitive on-site detection of Aflatoxin (AF) using surface enhanced Raman spectroscopy (SERS) and gold-coated superparamagnetic nanoparticles. **J. Neng***, J. Tan, P. Sun
- 380.** Route attribution of fentanyl using chemical attribution signatures. D. Mew, B. Mayer, A. Dehlope, **A.M. Williams Corrosion**
- 381.** Examination of optimization condition for electroless nickel plating process on copper. **N. Saito***, R. Suzuki, K. Noda
- 382.** Effect of ion species on dissolution behavior of Cu in acid solution. **K. Sawanobori***, R. Suzuki, K. Noda
- 383.** Effect of alloy elements on corrosion resistance of Co-Cr alloy. **R. Suzuki***, R. Hirata, K. Noda
- 384.** Electrochemical behavior in galvanized steel exposed under steel. **D. Yamana***, K. Noda
- 385.** Localized corrosion behavior of type 304 and 316 stainless steels under stress loading environment. **T. Izuhara**, K. Noda
- 386.** Surface reaction of stainless steel in atmospheric environment. **M. Abe***, Y. Hirohata, K. Noda
- 387.** Measuring method for corrosion behavior of metal material in low concentration solution. **Y. Yagi**, R. Suzuki, K. Noda
- 388.** Effect of oxide film thickness on corrosion of Ti. **K. Oniwa**, R. Suzuki, K. Noda
- Pharmacological and Biochemical Applications**
- 389.** Authentication of common Chinese medicine using Fourier Transform Infrared (FTIR) spectrometer. **M. Cheng***, T. Law, A. Singh, Y. Chan, S. Ip
- 390.** Membrane permeabilization and biological activity of fluoro-ixoprofen. **N. Yamakawa***, T. Mizushima
- 391.** Polyacrylamide gel electrophoresis oriented toward the identification of metalloproteins. **S. Saito***, M. Shibukawa
- 392.** Mannose-recognizable chemosensor using gold nanoparticles functionalized with pradimicin, a nonpeptidic mannose-binding natural product. **M. Enomoto***, Y. Igarashi, M. Sasaki, H. Shimizu
- 393.** imCorrect: New UHRS signal handling approach for more accurate elemental composition determination. **W. Chang***, Y. Huang*, Y. Chen
- 394.** Discrimination of *Polygonatum* species using ¹H NMR- and UPLC-QTOF MS-based metabolic profiling. **Y. Jung**, M. Lee, G. Hwang*
- 395.** Desorption electrospray ionization mass spectrometry (DESI-MS) as a tool for classification of pediatric brain tumors. **N.V. Schwab***, I.A. Cardinalli, P.H. Vendramini, M.N. Eberlin
- 396.** Mass spectrometer for skin-surface compounds using dual desorption/ionization plasmas. **M. Aida***, K. Kakegawa, T. Nagoya, H. Miyahara, Y. Seto, A. Okino
- 397.** Simple and versatile non-hybridization method for genetic diagnosis based on direct discrimination of single base mutation by capillary electrophoretic separation of single-stranded DNA. **T. Takahashi***
- 398.** Development of Thio-tag magnetic bead for rapid and selective separation of thiol-containing biomolecules. **M. Kawaguchi***, N. Koretake, E. Kinoshita-Kikuta, E. Kinoshita, T. Koike
- 399.** Protein separation technique using silica-based anion exchange chromatography. **T. Jikyo***, M. Kawai
- 400.** Comparing multistep IMAC and multi-step TiO₂ methods for comprehensive phosphopeptide enrichment. **X. Yue**, A.B. Hummon
- 401.** Chemical reaction induced multimolecular hyperpolarization technique for early-stage cancer diagnosis. **Y. Lee***
- 402.** Monitoring of 57 erectile dysfunction drugs and their analogs in foods and dietary supplements by LC-MS/MS. **S. Cho**, J. Lee, J. Jeong, H. Park, J. Do, S. Heo, J. Jo, S. Park, C. Yoon, S. Baek
- 403.** Peroxidase-like activity of natural iron corrosion powder and its application of H₂O₂ and glucose detection. **T. Kojima***
- 404.** Development of deep ultraviolet-excitation photothermal heterodyne-interferometer combined with capillary HPLC for label-free analysis of biologically-relevant molecules. **K. Aoki**, M. Isoda, A. Harata*
- 405.** Structural and functional analysis of E-cadherin-binding aptamer that forms parallel type G-quadruplex containing three long loops. **R. Maruyama**, K. Yoshimoto
- 406.** Thermodynamic stability of water-BSA-guanidine hydrochloride system. **R. Midorikawa***, T. Hanada, M. Takayanagi, A. Nagoe, T. Sugimoto, H. Fujimori

Wednesday Afternoon

Marriott Waikiki Beach
Waikiki Bllrm III

New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15)

Organized by: S. Krylov, D. Wilson, W. Zhong, H. Wang
Presiding: D.J. Wilson, W. Zhong

- 13:00** Opening statement on MS-based assays
- 13:05 – 407.** New MS tools for the discovery and characterization of protein-carbohydrate interactions. **J. Klassen**
- 13:35 – 408.** Native mass spectrometry of biomolecular complexes as a tool for protein structural biology. **J. Loo***
- 14:05 – 409.** Microdroplet fusion mass spectrometry for fast kinetic analysis. **J. Lee**, H. Nam, R.N. Zare*
- 14:25 – 410.** Quantitative mass spectrometric assessment of proteomic and phosphoproteomic changes that accompany exposure of human cells to low doses of ionizing radiation. X. Yue, A. Schunter, A.B. Hummon
- 14:45 – 411.** Using charge migration to probe interactions in the dissociation of gas-phase protein complexes. S. Fegan, M. Thachuk
- 15:05 Break**
- 15:20 – 412.** Lipid imaging of invertebrate model systems by mass spectrometry. **N.T. Phan***, A. Mohammadi, M. Dowlatshahi Pour, A.G. Ewing, J.S. Fletcher
- 15:40 – 413.** Higher order structural analysis of protein therapeutics by covalent labeling/mass spectrometry. N. Borotto, E. Graban, **R.W. Vachet***
- 16:00 – 414.** Paratope and epitope structural elucidation of antigen-antibody complexes using HDX and top/middle down subzero LC-ETD-MS/MS. **C.H. Borchers***
- 16:20 – 415.** Identifying how protein interactions alter the structure of parkin, an E3 ligase in early-onset Parkinson's disease. **G.S. Shaw***, J.D. Aguirre, T.E. Condros, K.R. Barber
- 16:40 – 416.** Time-resolved electrospray mass spectrometry (TRESI-MS) for dynamic characterization of function-related transitions in intrinsically disordered proteins. S. Zhu, P. Liuni, D. Resetcak, P. Gunning, **D.J. Wilson***

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Marriott Waikiki Beach
Kona Moku Blrm B

Current Issues in Teaching Analytical Chemistry (#38)

Organized by: T. Wenzel, C. Lucy, G. Dicinoski
Presiding: G. Dicinoski, C. Lucy, T. Wenzel

13:00 Introductory Remarks

13:05 – 417. The Analytical Sciences Digital Library - an electronic resource supporting problem-based learning. **C.K. Larive***
13:35 – 418. Development of E-learning modules that incorporate active learning exercises in the undergraduate analytical chemistry curriculum. **T. Wenzel**

14:05 – 419. Theoretical or technique classification in teaching analytical chemistry? A recent discussion in Chinese universities. **X. Zhang***

14:35 – 420. Threshold learning outcomes for undergraduate science degrees in Australia. **B.F. Yates***, S.M. Jones

15:05 Break

15:20 – 421. Teaching analytical chemistry in International College of Osaka University. **H. Watari***

15:50 – 422. "Jigsaw" classroom model and project-based labs in upper-division chemistry courses. **A.V. Krivoshein***

16:10 – 423. Effect of curricular restructuring and the implementation of the "flipped classroom" method on student engagement, outcomes, and retention in quantitative chemical analysis. **A.D. Marchetti***

16:30 – 424. Promoting the gradual development of process skills in analytical chemistry courses at a primarily undergraduate institution. **N.J. Ronkainen***

16:50 Concluding Remarks

Marriott Waikiki Beach
Milo III

Frontiers in Flow Injection Analysis and Related Techniques (#45)

Organized by: T. Imato, G. Christian, K. Grupan, S. Kolev, A. Sabarudin

13:00 – 425. Microfluidic droplet systems for high-throughput analysis and sensing: Updates on continuous flow analysis. **R. Kennedy**

13:25 – 426. Flow analysis based on optical devices fabricated by organic thin films. **T. Imato***

13:50 – 427. Spectrophotometric flow injection analyses for the inhibitory assay of xanthine oxidase and the assay of oxidant scavenging capacity. **T. Takayanagi***, A. Kimura, K. Matsumoto, T. Yabutani

14:15 – 428. Electrodialytic ion transfer for sample pretreatment, separation and pre-concentration for ionic solute analysis. **S. Ohira***, K. Nakamura, T. Yamasaki, P.K. Dasgupta, K. Toda

14:40 Break

14:55 – 429. Electrochemical flow-through cell fabricated with track-etched micro-porous membrane electrodes and its applications: flow analysis. **H. Mizuguchi***

15:20 – 430. Bringing flow injection analysis to the semantic web. **S.J. Chalk**

15:40 – 431. Organic polymer-based monolith for fast, efficient, and environmentally friendly separation of DNA sample. **A.N. Tasfiyat***, E. Malis, S.P. Sakti, E.D. Ifitah, A. Sabarudin*

16:00 – 432. Fusion of oil droplets in a microfluidic device using optical tweezers. **M. Mitsunobu**, S. Kobayashi, N. Takeyasu, T. Kaneta*

16:20 Closing Remarks

Marriott Waikiki Beach
Kona Moku Blrm C

Advances in Analytical Ion Mobility Separations (#61)

Organized by: A. Shvartsburg, F. Misaizu, T. Pukala
Presiding: T.L. Pukala

13:00 – 433. Ion mobility calculations using quantum mechanics and electronic surface representation for biological objects into the mega Dalton range. **Y. Alexeev***, J. Insley, D.G. Fedorov, A. Shvartsburg

13:30 – 434. Structures and CO-adsorption reactivities of nickel oxide cluster ions studied by ion mobility mass spectrometry. **K. Ohshima**, S. Azuma, T. Komukai, R. Moriyama, M. Nakano, F. Misaizu*

14:00 – 435. Advancing neuopeptidomic research via novel application of ion mobility mass spectrometry (IM-MS). **L. Li***, C. Jia, C. Lietz, Q. Yu

14:30 – 436. State-selective ion mobility in helium at very low temperature, isomer dependent mobility of small molecular ions in helium at room temperature, and theoretical model calculation of molecular ion mobility in air. **H. Tanuma**

15:00 Break

15:20 – 437. Geometrical structures of alkali-halide cluster ions investigated by ion mobility-mass spectrometry. **K. Ohshima**, T. Takahashi, R. Moriyama, M. Nakano, F. Misaizu*

15:50 – 438. Pharmaceutical applications of ion mobility spectrometry (IMS): Chemical reaction monitoring and isomeric analysis. **S.X. Li***

16:20 – 439. Determination of solid-derived fungal species by ion mobility spectrometric analysis of microbial volatile organic compounds for conservation technology of cultural heritage. **T. Takeuchi***, T. Kimura, M. Masuda, S. Tsuri, T. Suzuki, Y. Nakamura, T. Sugai, T. Akashi, H. Fujimiya

Marriott Waikiki Beach
Milo I

Immunoanalysis: Applications and Trends for Environmental Monitoring and Human Health (#94)

Organized by: S. Gee, I. Kennedy, H. Ohkawa, T. Xu, T. Papamontol
Presiding: S. Gee

13:00 – 440. Can nanobiotechnology fulfill in vitro diagnostic challenges?. **M. MARCO***

13:30 – 441. Multiplexed immunoensors for niche applications. **F.S. Ligler***, B.M. Cummins, G.M. Walker, M. Lochhead, C. Hammatt-Stabler, K. Caddell, J. Yeh

14:00 – 442. Molecular and cellular diagnostics via microfluidics biotechnology. **L. Qin***

14:20 – 443. Application for mycotoxin measurement in food using Q-body and quartz crystal microbalance. **Y. Sugita-Konishi***, T. Yoshinari, H. Ohashi, R. Abe, R. Kalgome, M. Wagatsuma, Y. Kamata, H. Ohkawa

14:50 – 444. Repetitive immunoensing with a highly stable protein monolayer and surface acoustic wave device for allergen monitoring. **K. Toma**, D. Miki, N. Yoshimura, K. Miyajima, T. Arakawa, H. Yatsuda, K. Mitsubayashi*

15:10 Break

15:25 – 445. Environmental monitoring by validated immunochemical methods. **N. AbdelShafy, C.Y. Vélez Montes, P. Carl, C. Knizia, H. Hoffmann, S. Schmidt, S. Andrade Roquette, L. Oberleitner, S. Gártner, R.J. Schneider***

15:45 – 446. Nanofield effect transistors-based label-free immunoensors. **A. Mulchandani**

16:05 – 447. Micro-optofluidic ELISA for rapid cytokine detection toward drug susceptibility test. **R. Usuba***, M. Yokokawa, A. Llobera, S. Murata, N. Ohkohchi, H. Suzuki

16:25 Concluding remarks

Marriott Waikiki Beach
Kona Moku Blrm A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung

Presiding: L. Baker, P.W. Bohn, S.C. Jacobson

13:00 Introductory Remarks

13:05 – 448. Bipolar electrode coupling of nanoscale electron transfer reactions to remote luminescent reporter reactions. **C. Ma, L. Zaino, D. Han, W. Xu, E. Foster, P.W. Bohn**

13:30 – 449. Thiol-ene-based microfluidic devices as versatile tools for pharmaceutical analysis. **J.P. Lafleur, A. Jönsson, S. Senkbeil, J.P. Kutter***

13:55 – 450. Nanopipettes as versatile tools for ion conductance measurements. **L. Baker***

14:20 – 451. Nanofluidic devices for characterizing virus capsids and their assembly products. **S.C. Jacobson***, Z.D. Harms, L. Selzer, A. Zlotnick

14:45 Break

15:00 – 452. Direct separation and analysis of cells mediated by transient molecular interactions in microfluidic devices. **R. Karnik***

15:25 – 453. Paper microfluidics: classic principles with new applications. **B. Lutz***

15:50 – 454. Hydrogel microengineering for biomedical applications. **S. Takeuchi***

16:15 – 455. Electrical single virus detection using transimpedance circuit integrated nanofluidic chip. **T. Yamamoto***

16:30 – 456. Digital microfluidic platform for UV-Vis absorbance spectroelectrochemistry. **M.D. Dryden***, A.R. Wheeler

Marriott Waikiki Beach
Waikiki Blrm II

Fundamentals and Applications of Atomic Spectrometry (#160)

Organized by: N. Furuta, G. Hieftje, R. Sturgeon
Presiding: C. Engelhard

13:00 – 457. Is there no better emission source than the ICP?. **G.M. Hiettje***, S.J. Ray, A.J. Schwartz, G. Chan, Y. Cheung

13:35 – 458. Extending the application range of provenance determination based on isotopic analysis. **F. Vanhaecke***, L. Balcaen, E. Boela-Fernandez, P. Degryse, V. Devulder, A. Gerdes, L. Lobo, A. Mage, M. Resano, A. Rua-Ibarz

14:10 – 459. Time-resolved spectroscopic studies of dielectric barrier discharges used as ambient desorption/ionization sources for mass spectrometry. **P.B. Farnsworth***, W.C. Ellis, M. Heywood, C. Reininger

14:45 Coffee break

15:05 – 460. Determination of Pu isotopic composition using SF-ICP-MS for radiation impact assessment of Fukushima nuclear accident released Pu in the marine environment. **J. Zheng***, T. Aono, K. Tagami, S. Uchida, M. Yamada

15:40 – 461. Arsenic speciation in food samples. **K. Chiba***, T. Narukawa

16:15 – 462. Improved sample introduction system for inductively coupled plasma spectrometry. **A. Al Hejami, T. Anderlini, D. Beauchemin***

Marriott Waikiki Beach
Milo IV / V

(Bio-)Chemical / Electrochemical Sensors and Sensing Materials (#417)

Organized by: K. Suzuki, P. Buhlmann, D. Citterio, O. Niwa, M. Winnik, K. Mitsubayashi

Presiding: E. Bakker, K. Suzuki

13:00 Opening remarks

13:05 – 463. Design of artificial bioluminescent probes towards bioluminescence imaging. **K. Suzuki***, R. Nishihara, S. Kim, T. Nakajima, M. Sato, D. Citterio, S. Nishiyama

13:20 – 464. New sensors and probes with ion-selective nanospheres. **E. Bakker***, X. Xie, J. Zhai

13:50 – 465. Fluorescent graphene oxide-based optical biosensor for the selective and sensitive detection of neurotransmitters. **S. Jeon**, S. Kwak, D. Yim, J. Ju, J. Kim*

14:10 – 466. Fluorescence sensing of double-stranded RNAs by triplex-forming peptide nucleic acid probes possessing thiazole orange as fluorescent universal base. **T. Sato**, Y. Sato, S. Nishizawa

14:30 – 467. Development and applications of "Mass Spectrometry Sensor" based on paper spray ionization of microdroplets. **J. Lin***, W. Liu

15:00 Break

15:10 – 468. Ligase-assisted signal-amplifiable DNA sensing using photon upconversion nanoparticles. **P. Wang**, T. Ozkaya Ahmadov, C. Lee, P. Zhang*

15:30 – 469. Ultrasensitive aptamer-based colorimetric and SPR biosensors for the detection of protein biomarkers, viruses, and small chemicals. **M. Gu***

15:50 – 470. Cavitas sensor and Sniff-camera for human biosensing. **K. Mitsubayashi**

16:20 – 471. Microbiosensor for the detection of methane in environmental samples. **Y. Chen**, Y. Zhang, T. Yu*

16:40 – 472. 3D cell co-culture platform on a microfluidic chip to mimic cancer niche and its application in multi-drug resistance research. **S. Wang***, J. Lin

Marriott Waikiki Beach
Waikiki Blrm I

Plasmonic Materials for Chemical Analysis (#450)

Organized by: D. Boudreau, J. Masson, A. Haes, J. Shumaker-Parry, M. Fan
Presiding: A.J. Haes

13:00 – 473. Plasmons as photonic intermediaries in redox photochemistry. **M. Moskovits***

13:40 – 474. Flexible plasmonic substrates for SERS detection of small molecules: The impact of adsorption equilibrium. **L. Tay***, J. Hulse, M. Laflamme, J. Fraser

14:00 – 475. Design and properties of anisotropic plasmonic materials. **A. Ianoul**

14:20 – 476. Controlling and designing plasmonic sensors at the single particle level. **E. Ringe***

14:40 – 477. Colloidal plasmonic metal nanocrystals. **J. Wang***

15:00 Health break

15:20 – 478. New methods in plasmonic biosensing: SPR phase imaging, nanoring/nanocone arrays, and single nanoparticle SPR microscopy. **R.M. Corn***

15:40 – 479. Grating-coupled propagating surface plasmon/localized plasmon hybrid excitations and their plasmonic device applications. **A. Baba***, K. Shinbo, K. Kato, F. Kaneko

* Principle Author

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- 16:00 – 480.** Probing the localized plasmon decay for nanostructures with complex geometries using atomic layer deposition. **C. Lancaster**, J.S. Shumaker-Parry
16:20 – 481. Imaging plasmons with compressive hyperspectral microscopy. L. Lu, L. Anderson, J. Hafner, **K.F. Kelly***
16:40 – 482. Surface-enhanced sensing and imaging analysis based on nanoplasmonic aperture arrays. **D. Kim**

Wednesday Evening

Marriott Waikiki Beach
 Kona Moku Ballroom A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung
 Presiding: Y. Baba, K. Otsuka, T. Yasui

19:00 – 483. Development of electroosmotic pumps based on materials for LC columns. **T. Naito**, A. Kunisawa, S. Futagami, T. Kubo, K. Otsuka

19:15 – 484. Molecular diffusion-based switching system using microelectrode array for evaluation of respiration activity of 3D cultured cells. **K. Ino**, Y. Yamada, H. Shiku, T. Matsue

19:30 – 485. Novel method of immobilizing antigens on gold electrode for immuno-sensing. **U. Nguyen**

19:45 – 486. Rapid and low-cost detection of epithelial growth factor receptor mutations in lung cancer cells. **T. Kasama***, T. Hase, N. Nishiwaki, N. Yogo, M. Sato, M. Kondo, N. Kaji, M. Tokeshi, Y. Hasegawa, Y. Baba

20:00 – 487. 2D control of ionic transport and electrochemical reaction in nanofluidics using a highly focused electric field of an electron-beam. **H. Miyazako***, K. Mabuchi, T. Hoshino

20:15 – 488. Electrical and optical detection of fine particulate matter ($PM_{2.5}$) based on microfluidic system for environmental monitoring assessment. **S. RAHONG**, T. Yasui, H. Yasaki, T. Yanagida, M. Kanai, K. Nagashima, N. Kaji, T. Kawai, Y. Baba

20:30 – 489. Detection of countable-number of molecules by integrating ELISA in extended-nano space. **R. Ohta***, K. Mawatari, K. Shirai, H. Shimizu, T. Kitamori

20:45 – 490. Metal ion sensor using thermo-responsive gel enclosing photonic crystal on a microchip. **K. SAGA**, K. Morikawa, T. Tsukahara *

Hawaii Convention Center
 Halls I, II, III

Fundamentals and Applications of Atomic Spectrometry (#160)

Organized by: N. Furuta, G. Hieftje, R. Sturgeon
 Presiding: N. Furuta

Poster Session

19:00 – 21:00

491. Particle to gas conversion and gas to particle conversion for analysis of atmospheric aerosols by ICP-MS. **T. Nakazawa**, R. Fukushima, N. Furuta*

492. Source apportionment of size-classified airborne particulate matter by multi-element fingerprinting. **A. Iijima***, H. Sato, A. Kuribara, S. Kudo, N. Furuta

493. Stability of silicic acid complex with positive ions in silica scale. **M. Tanaka***, H. Ariga, K. Takahashi

494. Elucidation of the origin of suspended particles in the Sumida River Estuary. **K. Uonomi**, T. Nakazawa, N. Furuta*

495. Novel approaches to improve preconcentration efficiency by using “bifunctional” extractant: Synthesis and application of 1-(dithiocarboxy)proline for preconcentration of trace elements by extraction/elution. **M. Murakami***, M. Hirano, K. Itoh

496. Sequential extraction and speciation of potentially toxic elements in sediments and water. **A.A. Ambushe***, T.W. Godeto

497. Speciation analysis of iodine in the Kanda River water by IC-ICPMS and ESI-MS. **H. Masuda**, T. Nakazawa, N. Furuta*

498. Speciation analysis of bromine in tap water by IC-ICPMS and ESI-MS. **M. Seto***, T. Nakazawa, N. Furuta

499. Development of undersized (12.5 mm diameter) glass beads for X-ray fluorescence determination of 34 components in 200 mg of igneous rock. **S. Ichikawa***, H. Onuma, T. Nakamura

500. Non-destructive and three-dimensional bulk analysis using high energy muonic X-rays for archaeological artifacts. **K. Ninomiya***, M.K. Kubo, T. Nagatomo, W. Higemoto, N. Kawamura, P. Strasser, K. Shimomura, Y. Miyake, S. Sakamoto, A. Shinohara, T. Saito

501. Analysis of arsenic in hair fraction by inductively coupled plasma-mass spectrometry. **S. Suzuki***, Y. Suzuki, M. Kasamatsu, Y. Seto

502. Element concentration in digestive gland and branchial hearts of cephalopods in East China Sea. **Y. Harada**, K. Tsuchiya, M. Tanaka*

503. Commercial development of a palladium isotope-based cell barcode for use in CyTOF cell assays. **D. Majonis***, M. Konrad, G. Wong, G. Behbehani, A. Terekidi, N. Qian, K. Askarpour, O.I. Ornatsky, V.I. Baranov, T. George, D.R. Bandura, S.D. Tanner

504. Application of ICP-MS to forensic discrimination of trace physical evidence. **M. Kasamatsu**, Y. Suzuki, S. Suzuki, Y. Seto

505. Sources of vermilion collected from ancient Japanese tombs, based on the trace elements and lead isotopes. **K. Takahashi***, T. Minami, S. Imazu, Y. Sahoo, M. Kitagawa, M. Kidera

506. Temporal changes in the fractionation index explained by the changes of size distribution of ablated particles. **R. Machida**, T. Nakazawa, N. Furuta*

507. Detection capability of laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) for elements from flame retardants in plastics. **M. Ohata***, Z. Yanbei, N. Itoh, T. Otake, N. Hanari

508. Precise and accurate determination of Sn in NIST 610 glass standard by laser ablation in liquid with isotope dilution ICPMS. **M. Fujiwara**, Y. Sakuraba, R. Machida, T. Nakazawa, N. Furuta*

509. High spatial resolution analysis of elemental concentrations in ferromanganese nodule using LA-ICP-MS. **J. Hirata**, M. Tanaka*

510. Study on hazardous elements in soils by using iron particles-assisted gas plasma induced by transversely excited atmospheric CO_2 laser. **A. Khumaeni**, Z. Lie, K. Kagawa

Hawaii Convention Center
 Halls I, II, III

Magnetoanalytical Science: Separation, Characterization and Imaging (#320)

Organized by: H. Watarai, I. Fritsch, C. Fuh
 Presiding: I. Fritsch, C. Fuh, H. Watarai

Poster Session
 19:00 – 21:00

511. Magnetic field effects on CVD growth process of single-walled carbon nanotubes. **Y. TAKASHIMA**, A. Hamasaki, J. Uchimura, A. SAKAGUCHI, S. Ozeki*

512. Cryogen-free 25T superconducting magnet for magneto-science. **K. Watanabe***, S. Awaji, H. Oguro

513. Development of anisotropic nanocomposite gel using a high magnetic field. **M. Yamato***, K. Suzuki, N. Hirota

514. Effect of amorphous region on crystalline orientation in Poly(L-lactide)/Poly(DL-lactide) blend films under magnetic field with annealing process.

R. NAKAYAMA, H. IKAKE, M. TAKADA, Y. MUROGA, K. KURITA, S. SHIMIZU, S. KURUMI, K. SUZUKI, K. TAKAHASHI, K. Watanabe

515. Effects of magnetic treatment water on silica gel formation. **K. Kaida**, S. Sasahara, A. Hamasaki, S. Ozeki*

516. Freezing potential of ionic liquids and magnetic field effects on it. **H. Otsuka**, A. Hamasaki, S. Ozeki*

517. Interaction between aluminium ion and glycolic acid under acidic conditions. **T. Taketadu***, M. Etou, Y. Okae, T. Yokoyama

518. Kinetic analysis of two-stage magnetic rotation for the uric acid crystal. **Y. Takeuchi***, E. Beaugnon , M. Iwasaka

Thursday Morning

Marriott Waikiki Beach
 Milo III

Development and Applications of Techniques for Electrochemical Analysis (#24)

Organized by: J. Chen, D. Arrigan, C. Hu, B. Liu, K. Maeda

8:00 Opening

8:05 – 519. Voltammetry at a single nano-electrode. **J. Chen***, K.J. Aoki

8:25 – 520. Polarography with dropping carbon fluid electrodes. **H. Tatsumi***

8:45 – 521. Dynamic behavior of electric double layer impedance. **K.J. Aoki**

9:25 – 522. Double layer effect on electrode kinetics affected by nanostructures on the electrode surface. **Y. Kitazumi***, O. Shirai, M. Yamamoto, K. Kano

9:45 – 523. Surface wave: Revisited. **M. Yamamoto**, K. Kano

10:05 Break

10:20 – 524. Investigations of interfacial electrochemistry in ionic liquids by SPM. **B. Mao***

10:40 – 525. Influence of electrode geometry on the voltammetric behaviour of the nanoholes electrode arrays. **M. Atighorestan***, A.G. Brolo

11:20 – 526. Instrumental considerations related to surface electrochemical processes occurring under potentiostatic and potentiodynamic conditions: The platinum oxide example. **J. van Drunen**, A. McMath, J. Kim, G. Jerkiewicz*

11:20 – 527. Voltammetric detection of Co and Ni in urine samples. **M. Wajrak***, W. Lonsdale, J. Mate

Hawaii Convention Center
 Halls I, II, III

Current Issues in Teaching Analytical Chemistry (#38)

Organized by: T. Wenzel, C. Lucy, G. Dicinossi

Poster Session

10:00 – 12:00

528. Development of a novel coffee roasting process using green coffee bean grinder for energy reduction. **h. Song**, S. Lee, J. Her, K. Lee

Hawaii Convention Center
 Halls I, II, III

Frontiers in Flow Injection Analysis and Related Techniques (#45)

Organized by: T. Imato, G. Christian, K. Grupan, S. Kolev, A. Sabarudin

Poster Session

10:00 – 12:00

529. Determination of trace phosphate by ICP/AES using novel polyallylamine type adsorbent packed in column.

T. Sumida*, Y. Yano, M. Yamashita, Y. Okazaki, H. Kawakita, T. Fukutomi

530. Microflow system using PDMS microchip with chemiluminescence detection for investigation of nanoparticle-metal interaction. **P. Inpota**, W. Jeamsaksri, W. Sripunkhai, P. Sunintaboon, P. Wilairat, D. Nacapricha, R. Chantiwas*

531. Application of a flow-injection spin-trapping ESR method for evaluating the alkoxy radical elimination capacity (AREC) of selected antioxidants. **A. Nakajima**, T. Yamashita, T. Yamaguchi, K. Kawai, Y. Miyake, K. Kanao, K. Tajima*

532. Quartz crystal microbalance sensing of catechin. **Y. Kobayashi***, T. Saito

533. Pretreatment of phosphorus compounds by electrogenerated cobalt(III) ions and its evaluation by flow injection analysis. **H. Tanaka**, H. Kubo, M. Takeuchi

534. Nitric acid gas generator. **S. Nakagawa**, H. Tanaka, M. Takeuchi*

535. Automatic on-line solid-phase extraction-ICP-MS exploiting sequential injection analysis for ultratrace vanadium determination in human urine sample. **A. Inoguchi**, A. Ayala Quezada, H. Murakami, N. Teshima*

536. Determination of gaseous isoprene by flow injection analysis with a fluorometric detection. **Y. Yoshino**, H. Murakami, N. Teshima*

537. Differentiating organic and conventional grown oregano using ultraperformance liquid chromatography mass spectrometry (UPLC-MS), headspace gas chromatography with flame ionization detection (headspace-GC-FID), and flow injection mass spectrum (FIMS) fingerprints combined with multivariate date analysis. **B. Gao**, L. Yu

538. A flow method for preparation of a gold nanoparticle-polyamide nanohybrid using reverse micelles adsorbed on glass surfaces. **M. Takemoto**, T.H. Hasanin, Y. Okamoto, S. Ishizaka, T. Fujiwara*

539. Use of a novel chromosensor and sequential injection system for fluorometric determination of mercury(II). **N. Choengchan***, A. Petchmanan, K. Chantalakhana, P. Thongyoo, D. Nacapricha

540. Electrochemical flow-through cell fabricated with nanohole shaped gold electrode. **N. Yoshikawa**, S. Sato, T. Sato, G. Hayakawa, M. Iiyama, H. Mizuguchi

541. On-line pretreatment flow injection system for direct and simultaneous measurement of iodide and creatinine in human urine. **J. Sitinurak**, P. Inpota, T. Mantim, N. Ratanavimarnwong, P. Wilairat, D. Nacapricha*

542. Development of the novel FRET substrate for β -secretase activity assay. **M. Adachi**, Y. Iida*

Marriott Waikiki Beach
 Milo I

Supercritical Fluid Chromatography (SFC) for Analysis and Purification (#53)

Organized by: L. Miller, A. Rajendran, T. Bamba

8:00 – 543. Advances in supercritical fluid chromatography. **L. Miller***

* Principle Author

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8:20 – 544. Correlation of retention factors for chiral separation in supercritical fluid chromatography in the presence of co-solvent. **T. Funazukuri***, T. Sugihara, Y. Ohno, M. Taguchi

8:50 – 545. Method-transfer in SFC - how similar is it to HPLC method-transfer strategies? **A. Tarafder***

9:20 – 546. Application of supercritical fluid chromatography (SFC) in contract research organization (CRO). **B. Su***

9:50 Break

10:00 – 547. Separation of polar biological compounds using enhanced-fluidity liquid chromatography, a subclass of sub-critical chromatography. **S. Olesik**, M. Beres, R. Bennett

10:30 – 548. Supercritical fluid chromatography triple-quadrupole mass spectrometry-based methodology for highly-sensitive and high-throughput analysis of multiresidue pesticides. **Y. Izumi**, E. Fukasaki, T. Bamba*

11:00 – 549. Application of SFE-SFC coupling for purification activities in drug discovery processes. **K. Gahm***

11:30 – 550. Development of novel Poly(vinylpyridine)-based SFC column. **K. Nagai**, S. Shinkura, T. shibata, A. Ohnishi

Hawaii Convention Center
Halls I, II, III

Advances in Analytical Ion Mobility Separations (#61)

Organized by: A. Shvartsburg, F. Misaizu, T. Pukala
Presiding: T.L. Pukala

Poster Session 10:00 – 12:00

551. Structure variation between vanadium oxide cluster cations and anions analyzed by ion mobility mass spectrometry. **J.W. Wu**, R. Moriyama, M. Nakano, K. Ohshima, F. Misaizu*

552. Ions of singly protonated enantiopure tryptophan, phenylalanine, and methionine in keV and eV collisions with chiral target gas. **M. Larson**, K. Kulyk*, O. Rebrov, M. Ryding, M. Stocket, J. Alexander, E. Ugerud, H. Cederquist

553. Structures and chemical compositions of gas phase chromium oxide cluster anions studied by ion mobility-mass spectrometry. **R. Moriyama**, R. Sato, T. Komukai, M. Nakano, K. Ohshima, F. Misaizu*

554. Structures and CO-adsorption reactions of cobalt oxide cluster ions investigated by ion mobility mass spectrometry. **M. Nakano**, R. Moriyama, K. Ohshima, F. Misaizu

Marriott Waikiki Beach
Kona Moku Blrm B

On-site and In-vivo Instrumentation and Applications (#88)

Organized by: J. Pawliszyn, G. Ouyang, M. Lee

8:00 Opening remarks

8:05 – 555. Liquid chromatographic instrumentation for on-site and point-of-care analysis. **M.L. Lee***, S. Sharma, A. Plistil, H.E. Barnett, S.D. Stearns, P.B. Farnsworth, A.J. Alpert, H. Tolley

8:25 – 556. Portable LC platforms: Concepts, technical issues, applicability. **Y. Li**, M. Dvorak*, N. Nuchtavorn*, P. Nesterenko*, R. Stanley*, **M. Macka***

8:45 – 557. Simple, flow-based quantitation of nucleic acid biomarkers in microfluidic devices. **A.T. Woolley***, D. Chatterjee, V. Sahore

9:05 – 558. Chip-scale sensors and handheld detector for real-time chemical vapor detection. **L. Zang***

9:25 – 559. Air monitoring of persistent organic pollutants with passive air samplers in King George Island, Antarctica. **Q. Zhang***, Y. Li, G. Jiang

9:45 – 560. Applying process analytical technology (PAT) tools to early active pharmaceutical ingredient (API) development. **S.X. Li***

10:05 Break

10:20 – 561. Online assessment of lubricant quality using fiber coupled fluorescence spectroscopy. **H. Lock***, N.L. Andrews, J.Z. Fan, H. Omrani, A. Dudelzak

10:40 – 562. Visible spectrometry with stacked transmission gratings. **A. Scheeline**

11:00 – 563. On-site instrument for automated monitoring of bacteria in water. **R. Brown***, C. Dunkinson, M. Douma, J. Zhou

11:20 – 564. In situ SERS detection of multi-class insecticides on plant surfaces. **L. He***

11:40 – 565. Real-time monitoring of fish stress response on threat behavior by using wireless biosensor system. **A. Aoki***, H. Wu, T. Arimoto, T. Nakano, T. Murata, H. Ren, H. Endo

Hawaii Convention Center
Halls I, II, III

Immunoanalysis: Applications and Trends for Environmental Monitoring and Human Health (#94)

Organized by: S. Gee, I. Kennedy, H. Ohkawa, T. Xu, T. Prapamontol
Presiding: S. Gee

Poster Session

10:00 – 12:00

566. Detection of influenza virus by an immunoassay combining liposome and electrochemiluminescence on Au electrode modified with binary self-assembled monolayers. **Y. Katayama***, Y. Mitoma, E. Hihumi, N. Egashira

567. Detection of influenza viruses by using oligonucleotide-based siRNA acid-modified nanoparticle. **D. Akamatsu**, M. Yamabe, Y. Ebara*

568. Develop ELISA KIT detecting melamine residues in feed and milk products in Vietnam. **H. Vu Thi***, A.Q. Bui*

569. Ultra highly sensitive detection of *Edwardsiella ictaluri* using high-gradient immunomagnetic separation with a polymerase chain reaction. **H. Wu***, K. Sugata*, H. Ohnuki, H. Ren, H. Endo

570. Isolating alpaca-derived V_HH antibodies to small molecule targets: Anecdotes from 7 experiments. **C.S. Bever**, J. Dong, Y. Cui, J. Wang, Z. Majkova, G. Gonzalez-Sapienza, S. Gee, B. Hammock

571. Highly sensitive SERS-based competitive immunoassay for detection of estradiol in human serum. **R. Wang**, J. Jeon, J. Choo*

572. Immunoanalysis of triclosan: Assay characterization, use and various formatting. **C.S. Bever**, A.A. Rand, K. Ahn, S. Gee, B. Hammock

573. Production of monoclonal antibody and development of an immunochromatographic assay for the rapid detection of histamine in fish samples. **L. Luo**, Z. Xu

574. Western blot with selective monoclonal antibodies induced by heat semi-denatured Bt Cry1Ac protein. **Z. Cao**, W. Zhang, B. Wang*

575. Synthesis of artificial antigens for four phthalate esters and determination by immunoassay. **D. Lai**, S. Zheng, S. Zhao

576. Highly sensitive immunoassay based on surface-enhanced Raman scattering for detection of bisphenol A. L. Zhang, S. Zhao

577. Particulate air pollution, dose response studies using particles of known composition. **G. Agnes**, S. Fenwick, X. Jia

Marriott Waikiki Beach
Kona Moku Blrm A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung
Presiding: H.J. Crabtree

8:00 Introductory Remarks

8:05 – 578. Microfluidic chip performance as a function of surface roughness. **H.J. Crabtree***, A. Ghobeity, M. Papini, J. Spelt

8:30 – 579. Silica-based microstructured fibers as customizable microfluidic conduits for chromatographic, electrophoretic, and mass spectrometric applications. **Y. Fu**, K. Bachus, G.T. Gibson, S. Morency, Y. Messaddeq, R.D. Oleschuk*

8:55 – 580. Miniaturised solventless electrophoretic sample enrichment and cleanup. **A. Wuethrich**, J. Quirino, P.R. Haddad*

9:20 – 581. IR transparent microfluidic devices. **C. Henry**, A. Krummel, S. Noblitt, B. Lehmkuhl, M. Barich

9:45 Break

9:55 – 582. Quantitative analysis of multiple microRNAs at the single-cell level. **S. Krylov**, W. David, F. Ghasemi

10:20 – 583. Using COTS materials to create cost-effective microfluidic systems using overhead transparencies and laser print, cut, and laminate fabrication. **J. Landers**, B. Thompson*, S. Krauss, J. DuVall, D. Haverstick

10:45 – 584. High throughput, microfluidic inertial migration-based cyanobacteria concentrator. **L. Wang**, D.S. Dandy

11:00 – 585. One-step modification and structuring of PDMS surfaces and its application in the bench-top fabrication of self-driven microfluidic channels. **A. Fatona**, Y. Chen, M.A. Brook, J. Moran-Mirabal*

11:15 – 586. Solid phase extraction of large volume samples on a flow-through centrifugal microfluidic devices. **E.J. Templeton**, C. Skinner, E.D. Salin*

11:30 – 587. High-throughput screening at the picoliter scale by combining dip pen lithography with inkjet printing. **G. Arrabito**, F. Cavalier, V. Vetrí, S. Di Maro, S. Cosconati, E. Novellino, C. Pellerito, V. Milletto, M. Leone, B. Pignataro*

11:45 – 588. OMVCD grown AuNPs on polymers substrates for biosensing application. **S. Mittler***, S. Kandepan

Marriott Waikiki Beach
Waikiki Blrm II

Fundamentals and Applications of Atomic Spectrometry (#160)

Organized by: N. Furuta, G. Hieftje, R. Sturgeon
Presiding: N. Furuta

8:00 – 589. Recent advances in mass cytometry. **D.R. Bandura***, O.I. Ornatsky, D. Majonis, T. Closson, M. Sullivan, A.V. Loboda, Y. Wei, V.I. Baranov, S.D. Tanner

8:35 – 590. Characterization and detection of nanoparticles using ICP-MS. **H. Lim***

9:10 – 591. Selenium and mercury speciation in blue tilapia from an aquaponic system. **S. Smith**, M. Schmale, J. Caruso, K. Savage, G. Delaney, J. Devin, J. Boenker, M. Shank, J. Landero-Figueroa

9:45 Coffee break

10:05 – 592. Investigation of different sample introduction systems for the analysis of discrete sample volumes using ICP-TOFMS. **D. Guenther***, A. Graham Gundlach, B. Hattendorf, L. Hendricks

10:40 – 593. ICP-MS based strategies for the analysis of trace metals and biomarkers in cells. **B. Hu**, B. Chen, M. He

11:15 – 594. Liquid sampling-atmospheric pressure glow discharge (LS-APGD) microplasma: Addressing diverse challenges in both OES and MS analysis. **R. Marcus***, L. Zhang, S. Jones, E. Hoegg

Marriott Waikiki Beach
Kona Moku Blrm C

Ultrasensitive Assays for Proteins and Protein Modifications (#287)

Organized by: C. Le, H. Zou, N. Dovichi
Presiding: C. Le, F. Li

8:00 – 595.

Femtogram proteomics: Bottom-up analysis of *E. coli* tryptic digests. **N. Dovichi***, L. Sun, G. Zhu, Y. Zhao, S. Mou, X. Yan, M. Champion

8:40 – 596. Cellular heterogeneity measured via high-throughput single cell mass spectrometry imaging and profiling. **J.V. Sweedler***, T. Ong, M.A. Makrath, E.T. Jansson, T. Comi, S.S. Rubakhin

9:20 – 597. Using mass spectrometry to understand posttranslational modifications in the misfolding of the cystic fibrosis transport regulator (CFTR). **J.R. Yates***, S. Pankow, C. Bamberger

10:00 – 598. Proteome identification goes deep and fast while quantification goes accurate and precise. **Y. Zhang**

10:40 – 599. High sensitivity mass spectrometry assays of disease-induced post-translational modifications. **J.E. Van Eyk***, Q. Fu, Z. Chen

11:20 – 600. Array-mass spectrometry hybrid platform to analyze protein modifications. **W.A. Tao***

Marriott Waikiki Beach
Waikiki Blrm III

Advances in FTIR Microspectroscopy: 3D Tomography to Nanoscale Imaging (#315)

Organized by: K. Gough, M. Martin, M. Chen
Presiding: K.M. Gough, M.C. Martin

8:00 Introduction

8:02 – 601. From nano-FTIR spectroscopy toward infrared nanotomography. **R. Hillenbrand**

8:32 – 602. Combining SINS at the ALS: Ultrabroadband infrared nanospectroscopy and imaging. **H.A. Bechtel**, E. Muller, M.C. Martin, M.B. Raschke

9:02 – 603. Observations of a core-shell structure in single electrospray poly[(R)-3-hydroxybutyrate-co-(R)-3-hydroxyhexanoate] (PHBHx) nanofibers by AFM-IR spectroscopy and imaging. **J.F. Rabolt***, L. Gong, B. Chase, I. Noda

9:32 – 604. Understanding heterogeneity in plasmonic metal oxide nanocrystals. **D.J. Milliron**, R. Johns, A. Agrawal, H.A. Bechtel

10:00 – 605. Introducing nano-FTIR: Imaging and spectroscopy at 10nm spatial resolution. **T. Gokus***, F. Huth, A. Huber

10:20 Break

10:30 – 606. Infrared nanospectroscopy, a high resolution tool to explore chromatin composition. **B.R. Wood***, E. Lipiec, W. Kwiatek, J. Miszyk, F. Ruggeri, G. Dietler, C. Adiba, A. Kulik

* Principle Author

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- 11:00 – 607.** Infrared spectral tomography: 3D IR images now in full color.
M.C. Martin*
- 11:20 – 608.** Mosaic tomographic imaging of individual cells employing a novel tomography accessory for infrared microscopes. **C.R. Findlay**, N. Pogorzelec, C. Mundy, K.M. Gough*
- 11:40 – 609.** Synchrotron infrared 3D confocal spectral imaging based on nonlinear reconstruction algorithm. **M. Chen***, H. Zhu, Y. Tong, T. Ji, W. Peng, Z. Zhang, T. Xiao

Marriott Waikiki Beach
Milo IV / V

(Bio-)Chemical / Electrochemical Sensors and Sensing Materials (#417)

Organized by: K. Suzuki, P. Buhlmann, D. Citterio, O. Niwa, M. Winnik, K. Mitsubayashi

Presiding: P. Buhlmann, O. Niwa

8:00 – 610. Curcubit[n]uril-functionalized water-stable FET sensors. **I. Hwang***, K. Kim*

8:20 – 611. Electrochemical sensing in biological samples with fluorous receptor-doped membranes. A.J. Dittmer, **P. Buhlmann***

8:50 – 612. Electrochemical lipopolysaccharide detection using zinc complex-based probes and sputtered nanocarbon film electrode. **D. Kato***, Y. Suzuki, K. Yoshioka, T. Kamata, S. Sasaki, M. Todokoro, O. Niwa

9:10 – 613. Coreactant-free and supersensitive sensing for Cu²⁺ by graphene oxide amplified electrochemiluminescence of graphitic carbon nitrid. **B. Xia**

9:30 – 614. Fabrication of patterned graphene electrode with a transfer process assisted by a polyimide thin film. **Y. Ueno***, K. Furukawa, T. Teshima, M. Takamura, H. Hibino

10:00 Break

10:10 – 615. Impedimetric detection of telomerase activity in cancer cells. **D.C. Diaz-Cartagena***, L. Cunci, E.M. Diaz-Diaz, M. Martinez-Vargas, C.I. Gonzalez, C.R. Cabrera

10:30 – 616. Graphene/polymer nanocomposites for sensitive biomolecular detection and medical diagnostics. **N. Rodthongkum***

10:50 – 617. Novel nitric oxide (NO) release materials/methods that improve the biocompatibility/antimicrobial activity and in vivo analytical performance of intravascular electrochemical sensors. **M.E. Meyerhoff***, A.K. Wolf, H. Ren, Y. Qin, X. Wang, K. Cha, W. Wen

11:20 – 618. Collagen/graphene nanocomposite-based sensor for enantiomer-recognition of chiral molecules. **R. Mohd Zawawi***, B. Kasinathan

11:40 – 619. Electrochemiluminescence biosensor for detection of cancer biomarkers on bipolar electrode array chip. M. Wu*, H. Chen*, **J. Xu***

Marriott Waikiki Beach
Waikiki Blrm I

Plasmonic Materials for Chemical Analysis (#450)

Organized by: D. Boudreau, J. Masson, A. Haes, J. Shumaker-Parry, M. Fan
Presiding: M. Fan

8:00 – 620. Smart enzymatic Ag/Au bimetallic nanoshells for nanoplasmonic bio-sensing. **Y. Jin***

8:40 – 621. Enhanced SPR measurements for the detection of clinically relevant molecules in crude biofluids. **K.S. McKeating**, J. Masson*

9:00 – 622. Metal decorated cellulose nanocrystals: A water dispersible SERS substrate. **M. McDermott**, R. Du

9:20 – 623. Detection of influenza virulence biomarkers by SERS. **R.A. Diluyi**

9:40 – 624. Selective plasmonic enhancements for molecular detection. **Z.D. Schultz***

10:00 Health break

10:20 – 625. Microdialysis SPR: Sensing in whole blood and biofluids. **J. Masson**, J. Breault-Turcot

10:40 – 626. Dialing up refractive index sensitivity: Compositional control within bimetallic plasmonic materials. **A.F. Smith***, R.G. Weiner, S. Harvey, S.E. Skrabala

11:00 – 627. Ex-situ and in-situ single-particle monitoring of temperature-dependent structural evolution in galvanic replacement reactions. **Y. Park**, c. Lee, S. Ryu, H. Song*

11:20 – 628. Listening to proteins with extraordinary acoustic Raman (EAR). **R. Gordon**

11:40 – 629. Gold nanoparticle-polymer sensor arrays for biomedical applications. **V.M. Rotello***

Thursday Afternoon

Marriott Waikiki Beach
Kona Moku Blrm A

New Tools and Methodologies for the Characterization of Biomolecular Interactions (#15)

Organized by: S. Krylov, D. Wilson, W. Zhong, H. Wang

Presiding: S. Krylov, D.J. Wilson

13:00 – 630. Focal mography: Coherent detection of biomolecular interactions. **C. Fattinger***

13:30 – 631. Single-molecule mechano-chemical sensing. **H. Mao***

14:00 – 632. Beyond the image: Napping protein interactions and oligomerization in living cells using fluorescence fluctuation and single molecule methods. **P.W. Wiseman***

14:20 – 633. Novel optical detection system for monitoring dissolved oxygen quenched-fluorescence and materials movements caused-deflection in plant activities. **X. Wu***, X. Wu, T. Inoue, H. Kubo

14:40 – 634. New structural bioinformatics tools to characterize interactions in biomacromolecular complexes based on large database data. **J. Koca***, R. Svoboda Varekova, D. Sehnal, C. Ionescu, S. Geidl, L. Pravda, D. Jaiswal, V. Horsky, M. Wimmerova

15:00 – 635. Atomic force microscopy for immunohaematology. **N. Yeow***, R. Tabor, G. Garner

15:20 – 636. General steric trapping strategy reveals an intricate cooperativity network in the intramembrane protease GlpG under native condition. **R. Guo**, K. Gaffney, X. Huang, H. Hong*, Z. Yang, M. Kim, W. Hubbell

15:40 – 637. Spatial distribution of nano-scale flexible chains as a protein terminal model visualized by 3D scanning force microscopy. **H. Asakawa***, K. Takao, N. Inada, T. Fukuma*

16:00 – 638. Detection of temperature, pH value and several biocomponents in vivo with novel fluorescent probes based on triaryl boron compounds and other intra-molecular charge transfer compounds. **G. Yang**

16:20 – 639. Peptide-water crystal studies using THz wave techniques. **D.F. Plusquellec**

Marriott Waikiki Beach
Milo III

Development and Applications of Techniques for Electrochemical Analysis (#24)

Organized by: J. Chen, D. Arrigan, C. Hu, B. Liu, K. Maeda

13:00 – 640. Theoretical prediction of the Gibbs energy of transfer of organic ions across the oil/water interface. **T. Osakai**

13:30 – 641. Manipulating and detecting ions in confined spaces for novel electroanalytical methodologies. **E. Bakker**, M. Cuartero, M. Ghahraman Afshar, G. Crespo

14:00 – 642. Reductive deposition of gold nanofibers at the liquid-liquid interface between highly hydrophobic ionic liquid and water. **T. Kakinami***, N. Nishi, K. Amano, T. Sakka

14:20 – 643. Electrochemical surface plasmon resonance to probe structure dynamics and electrochemical reactions at ionic liquid interface. **N. Nishi***, Y. Ikeda, K. Amano, T. Sakka

14:40 – 644. Electrolytic extraction of ionic species using the thin layer electrolysis cell for the ion transfer at the liquid/liquid interface. **Y. Yoshida***, J. UCHIDA, K. HOSOYA, K. Maeda

15:00 – 645. Propagation and synchronization of potential oscillations between two oscillation sites in the liquid membrane system. Y. Yamaguchi, Y. Yoshida, K. Maeda*

15:25 Break

15:40 – 646. Salt on a chip: miniaturised ionic liquid systems. **C. Zhao**, C. Gunawan, M. Ge, R. Gondoswanto

16:00 – 647. Effect of concentration and current density on zinc electrodeposition in ionic liquid electrolyte including bromide anion at high temperature. **C. Li**, K. Nishikawa, J. Moon, K. Kanamura

16:20 – 648. Nitrogen-doped graphene conductive catalyst for highly efficient dye-sensitized solar cells. **H. Chen***, E. Bi, X. Yang, L. Han

16:40 – 649. Formation of the SERS-active substrate and its application in catalysis and analytical detection. **J. Zhao**, K. Zhang, J. Ji, B. Liu*

Marriott Waikiki Beach
Milo I

Supercritical Fluid Chromatography (SFC) for Analysis and Purification (#53)

Organized by: L. Miller, A. Rajendran, T. Bamba

13:00 – 650. Application of supercritical fluid chromatography/mass spectrometry to metabolic profiling. **T. Bamba***

13:30 – 651. Advantages of supercritical fluid chromatography are more than green chemistry. **L.T. Taylor**, M. Ashraf-Khorassani

14:00 – 652. Combining the expertise of academics, industries, and manufacturers to develop an achiral SFC-MS screening strategy for impurity profiling of drug candidates. **C. West**, E. Lemasson, S. Bertin, H. Boiteux, P. Hennig, E. Lesselier

14:30 – 653. Marriage of SFC and mass spectrometry: An old romance rekindled. **J. Van Antwerp**

15:00 Break

15:15 – 654. Preparative phospholipid fractionation using near- and supercritical fluid chromatography. **F. Montanes***, S. Tallon

15:45 – 655. Separation of closely related pharmaceuticals by supercritical fluid chromatography in support of organic synthesis. **E.L. Regaldo***, C. Welch

Marriott Waikiki Beach
Kona Moku Blrm B

On-site and In-vivo Instrumentation and Applications (#88)

Organized by: J. Pawliszyn, G. Ouyang, M. Lee

13:00 – 656. In situ, in vivo characterisation of human tissues and associated microbiota by rapid evaporative ionization mass spectrometry – the iKnife. **Z. Takats***

13:25 – 657. Miniature mass spectrometry systems for analysis of tissue and biofluid samples. **Z. Ouyang***, Y. Ren, X. Wang, R. Zou, Y. Su, Y. Xia, R.G. Cooks

13:45 – 658. Sub-millimeter linear ion traps to address space-charge limits in portable mass spectrometry. **D. Austin**

14:05 – 659. Detection of gaseous compounds by needle trap sampling and direct thermal-desorption photoionization mass spectrometry: Concept and demonstrative application to breath gas analysis and ship exhaust. **R. Zimmermann**, J. Kleebatt, J. Schubert, T. Streibel

14:25 – 660. Robust and compact active capillary plasma ionization source: design and applications. **R. Zenobi***

14:45 – 661. Chemical biopsy based on SPME approach: A new medical tool. **J. Pawliszyn**

15:05 Break

15:20 – 662. Determination of chemicals in individual small organisms and single cells using nanolayer probe. **T. Luan***

15:40 – 663. In situ analysis of volatile and semi-volatile organic compounds with applications for geospatial mapping of atmospheric contaminants by membrane introduction mass spectrometry. N. Davey, R. Bell, L. Richards, D. Letourneau, M. Angelstad, C.G. Gill, **E.T. Krogh***

16:00 – 664. Fast quantification of transformation products of rocket fuel unsymmetrical dimethylhydrazine in soil using solid-phase microextraction and GC-MS. N. Bakaikina, **B. Kenessov***, S. Yegemova, J. Koziel

16:20 – 665. Monitoring of persistent organic pollutants in seawater of the Pearl River estuary with rapid on-site active SPME sampling technique. **G. Ouyang***

16:40 – 666. Monolithic materials for rapid sample preparation. **E. Hilder**, E. Candish, R.A. Shellie, H. Wirth, A. Gooley

Marriott Waikiki Beach
Waikiki Blrm II

Fundamentals and Applications of Atomic Spectrometry (#160)

Organized by: N. Furuta, G. Hietjje, R. Sturgeon

Presiding: S.J. Ray

13:00 – 667. Laser ablation molecular isotopic spectroscopy (LAMIS). **R.E. Russo***

13:35 – 668. Coupling of multiscale imaging and high resolution U-Pb chronology. **T. Hirata***, S. Sakata, K. Hattori, T. Suzuki

14:10 – 669. Analysis of trace metals in open ocean seawater samples using resin based extraction methods with sector field ICP-MS detection. **A. Townsend***, F. Queroue, P. van der Merwe, D. Lannuzel, G. Sarthou, A. Bowie

14:45 Coffee break

15:05 – 670. Real time monitoring of multi-elements concentration in airborne nanoparticles (ANPs) by direct introduction into ICP-MS. **N. Furuta***, R. Fukushima, T. Nakazawa

15:40 – 671. Use of polymer inclusion membranes (PIM) for online separation in flow analysis. **S.D. Koley***

16:15 – 672. Laser ablation ICP-MS for application in elemental microscopy with sub-micrometre resolution. **N. Jakubowski***, H. Traub, D. Esteban-Fernandez, R. Hutchington, C. O'Connor

* Principle Author

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Marriott Waikiki Beach
Kona Moku Blrm C

Ultrasensitive Assays for Proteins and Protein Modifications (#287)

Organized by: C. Le, H. Zou, N. Dovichi
Presiding: C. Le, H. Zhang

13:00 – 673. Microfluidic system for western blotting. **R. Kennedy**

13:40 – 674. High peak capacity, 2D separations using micro free flow electrophoresis. **M.T. Bowser***, M. Geiger, A. Johnson, S. Anciaux

14:20 – 675. Integrative approach to identify metalloproteomes in microbes. **H. Sun**, H. Wang, Y. Wang, L. Hu

15:00 Break

15:20 – 676. Quantum dots and upconversion nanoparticles as active elements in optical sensing for development of sensitive solid-phase protein and oligonucleotide bioassay platforms. **U. Krull***, S. Doughan, M. Noor, U. Uddayasanarkar, A. Shahmurdyan, F. Zhou, Y. Han

16:00 – 677. Plant-derived natural product restores activity of mutant ph enylalanine hydroxylase: A novel pharmacological chaperone for treatment of phenylketonuria. **P. Britz-McKibbin***, M. Shanmuganathan

16:40 – 678. Binding-induced DNA nanomachines triggered by proteins and nucleic acids. **H. Zhang***, J. Chen, B. Deng, X. Li, C. Le*

Marriott Waikiki Beach
Waikiki Blrm III

Advances in FTIR Microspectroscopy: 3D Tomography to Nanoscale Imaging (#315)

Organized by: K. Gough, M. Martin, M. Chen
Presiding: M. Chen, K.M. Gough

13:00 – 679. Synchrotron FTIR imaging initiatives at CLS Beamline 01B1-1. **S.M. Rosendahl***

13:25 – 680. Application and perspective of FTIR microspectroscopy on the characterization of animal silks and silk protein-based materials. **X. Chen***, S. Ling, G. Fang

13:55 – 681. IR spectroscopic analysis of oceanic phytoplankton blooms performed for the first time on board a ship. **P. Heraud***, O. Sackett, K. Petrou, J. Beardall

14:15 Break

14:25 – 682. Investigating quantum cascade laser based infrared for rapid clinical diagnostics. **M. Baker***, C. Hughes, G. Clemens, B. Bird

14:55 – 683. Quantum cascade laser mid-IR imaging: Giving real-time biochemical feedback to the pathologist. V. Varma, H. Sreedhar, P. Nguyen, B. Davidson, A. Husain, G. Guzman, S. Setty, M.J. Walsh

15:15 – 684. Challenges of scale in the FTIR spectrochemical imaging of biological samples. **K.M. Gough***, C.R. Findlay, M. McLellan, R. Wiens

15:45 – 685. Laser-based mid-infrared chemical imaging. **M. Barre***, E. Fotheringham, B. Bird, B. Mohar, M. Weida, D. Arnone, J. Rowlette

16:05 – 686. Infrared hyperspectral imaging of biomedical samples using high magnification optics. C. Hughes, M. Pilling, A. Henderson, M. Jimenez-Hernandez, P. Bassan, M. Kansiz, K. Dorling, M. Brown, N. Clarke, **P. Gardner***

16:35 Closing discussion

Marriott Waikiki Beach
Milo IV / V

(Bio-)Chemical / Electrochemical Sensors and Sensing Materials (#417)

Organized by: K. Suzuki, P. Buhlmann, D. Citterio, O. Niwa, M. Winnik, K. Mitsubayashi
Presiding: D. Citterio, K. Mitsubayashi, M. Winnik

13:00 – 687. Label-free sensor array chips: Application to simultaneous RNA sequence detection. **H. Aoki***

13:20 – 688. Building an imaging toolbox: Optical nanosensors for biological discovery. **H.A. Clark***, W. Di, A. Sahari, E. Hondroulis

13:50 – 689. New-generation enzyme-free hydrogen peroxide amperometric sensor based on ZnS:Mn/graphene nanocomposites. **D. Diaz***, J. Beltran-Huarac, B.R. Weiner, G. Morell

14:10 – 690. Integration of SERS-based nanostress sensing with microcontact printing provides sensitive multiplex detection of liver cancer biomarkers. **M. Li**

14:30 – 691. Spontaneously blinking fluorophore based on intramolecular spirocyclization for live-cell super-resolution imaging. **Y. Urano***

15:00 Break

15:10 – 692. Glucose metabolism sensors for the extracellular and intracellular assays. **L. Zhang***, F. Su, X. Kong, S. Buizer, F. Lee, K. Day, Y. Tian, D.R. Meldrum

15:30 – 693. eSHHA homogeneous platform: Quantitative detection of biomarkers directly in whole blood. **S.S. Mahshid**, A. Vallée-Bélisle*

15:50 – 694. Ratiometric bioimaging and biosensing of reactive oxygen species and related biological species. **Y. Tian**

16:20 – 695. Development of fluorescent reagents for the detection of biological substances such as proteins and glycoconjugates. **T. Suzuki***, Y. Chiba, A. Kuno, O. Niwa

16:40 – 696. Biomimetic MIP thin films for bulk acoustic wave vapor sensors. **N. IQBAL***, A. Afzal, A. Mujahid

Marriott Waikiki Beach
Waikiki Blrm I

Plasmonic Materials for Chemical Analysis (#450)

Organized by: D. Boudreau, J. Masson, A. Haes, J. Shumaker-Parry, M. Fan
Presiding: J.S. Shumaker-Parry

13:00 – 697. Surface-enhanced Raman scattering tags and SHINERS. **C. Murphy***

13:40 – 698. Application of nanoparticles exhibiting metal-enhanced fluorescence for biochemical sensing. **D. Boudreau**, J. Asselin, M. Drouin, F. Laviole

14:00 – 699. Super-resolution imaging of fluorescently-labeled ligands bound to plasmonic nanostructure. **K. Willets**

14:20 – 700. Plasmonic spectroelectrochemistry—an advanced tool for rapid sensing and point-of-care diagnostics. **C.L. Brosseau***, L. Zhao, R. Karaballi, S. Harroun, J. Blackburn

14:40 – 701. Phospholipid bilayer encapsulated nanoparticles for SERS. **G. Walker***

15:00 Health break

15:20 – 702. Plasmonic optical tweezer for analytical chemistry. **Y. Tsuboi**

15:40 – 703. Developing shape adaptable surface enhanced Raman scattering (SERS) substrates for surface contamination analysis. **M. Fan**

16:00 – 704. Chemical sensing with refractive index sensitive plasmonic nanostructures. **T. Sannomiya***

16:20 – 705. Plasmonic enhancement and artificial receptor recognition for the detection of drugs. **A.J. Haes***, W. Xi

16:40 – 706. Membrane surface-enhanced Raman spectroscopy for sensitive detection of molecular behavior of lipid assemblies. **K. Suga**, **T. Yoshida**, H. Ishii, Y. Okamoto, H. Umakoshi*

Thursday Evening

Hawaii Convention Center
Halls I, II, III

Supercritical Fluid Chromatography (SFC) for Analysis and Purification (#53)

Organized by: L. Miller, A. Rajendran, T. Bamba

Poster Session

19:00 – 21:00

707. Supercritical fluid chromatography-mass spectrometry (SFC-MS) for the rapid simultaneous determination of 16 European priority polycyclic aromatic hydrocarbons in coffee beverage and black beer. **T. Yoshioka**, Y. Nagatomi, K. Harayama

708. Lipoprotein analysis of plasma lipoprotein fractions in myocardial infarction-prone rabbits. **H. Takeda**, T. Koike, Y. Izumi, T. Yamada, M. Yoshida, M. Shiomi, E. Fukasaki, T. Bamba*

709. Removal of endotoxin from DNA solution by cyclodextrin-urethane copolymer adsorbent. **M. Sakata***, T. Matsuo, M. Todoko

710. Rapid in-depth regiosomer focused lyophilophospholipids of human serum by online supercritical fluid extraction-super-critical fluid chromatography tandem mass spectrometry. **Y. Izumi**, M. Nakao, N. Tucket, Y. Funada, T. Uchikata, Y. Iwata, M. Tomita, N. Masayuki, K. Ekoos, T. Bamba*

711. Chiral separation of dextromethorphan/levomethorphan in hair samples by supercritical fluid extraction combined with ultra performance supercritical fluid chromatography-tandem mass spectrometry. **R. Kikura-Hanajiri***, K. Yamada, T. Hakamatsu

Hawaii Convention Center
Halls I, II, III

On-site and In-vivo Instrumentation and Applications (#88)

Organized by: J. Pawliszyn, G. Ouyang, M. Lee

Poster Session

19:00 – 21:00

712. Study of a method for analysis of trace elements in vegetables using a portable total reflection X-ray fluorescence spectrometer. **T. Yokoyama***, S. Kunimura

713. Advances in ion chromatography: New applications in CCS. **G. Fytianos***, H. Knuttila, H.F. Svendsen

714. In situ determination of arsenic in water by handheld X-ray fluorescence spectrometry. **K. Hagiwara**, Y. Koike, M. Aizawa, T. Nakamura*

715. Study of sample preparation methods for trace elemental analysis of various samples using a highly sensitive portable total reflection X-ray fluorescence spectrometer. **S. Kunimura***, S. Kudo, K. Suzuki, Y. Hojo, K. Amagasu

716. On-site determination of trace cadmium in environmental fresh water with 5,10,15,20-tetraphenyl-21H,23H-porphyrinetetrasulfonic acid. **S. Kawakubo***, Y. Sasaki, N. Yamamoto, Y. Suzuki, I. Ueta

717. Direct, on-line, in-situ/in-vivo quantitation of low volatility aqueous analytes in complex samples. Condensed phase membrane introduction mass spectrometry (CP-MIMS). K.D. Duncan, G. Vandergrift, D.A. Volmer, A. Cappiello, E.T. Krogh, **C.G. Gill***

718. Development of an optical transmission type biosensor for real-time monitoring of fish stress. **R. Shinoda***, H. Wu, T. Murata, H. Ohnuki, H. Ren, H. Endo

719. Environmental fates of synthetic musks in animal and plant: An in vivo study. **F. Zhu***, G. Chen, R. Jiang, G. Ouyang

720. Study of an appropriate sample holder for elemental analysis of particulate matter 2.5 using a portable total reflection X-ray fluorescence spectrometer. **Y. Matsumoto***, S. Kunimura

721. In-vivo fluorescence probes for real-time management of cyanobacterial blooms in water treatment plants. **A. Zamaydi***, F. Choo, G. Newcombe, R. Stuetz, R.K. Henderson

722. On site monitoring of methanethiol and dimethyl sulfide in Lake Baikal water and atmosphere. **K. Toda***, V. Obolkin, T. Nagahata, S. Iyadomi, N. Hozumi, S. Ohira, V. Potemkin, T. Khodzher

723. Development of simple analysis using smart device based on autocatalytic reaction with Na₂SO₃ and H₂O₂ followed by oxidase reaction. **M. Kurimoto**, A. Manaka*, S. Furuyama

Marriott Waikiki Beach
Kona Moku Blrm A

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung

Presiding: H.J. Crabtree, S.C. Jacobson, J. Ramsey

19:00 – 724. Lab-on-a-chip for monolith-based preconcentration and separation of phosphopeptides. M. Araya-Farias, S. Dziomba, F. Bayle, M. Guerrouache, M. Woytasik, H. Cao, B. Carbonnier, M. Taverna, **t. Tran-Maignan**

19:15 – 725. Label-free real-time measurement of protease activity by nanopore analysis. **X. Guan***, L. Wang, S. Zhou, X. Chen

19:30 – 726. Plasma-on-chip device for analyzing interactions between plasma gas and individual cells. C. Chang, J. Jeong, M. Kobayashi, T. Shimizu, M. Sasaki, **S. Kumagai***

19:45 – 727. Fabrication of nanoscale graphene field effect transistor biosensor for nucleic acid detection. **G. Zhang***, Y. Ning*

20:00 – 728. Site-specific working inside nanofluidic channels: General methodology, critical techniques, and nanobio applications. **Y. Xu***

20:15 – 729. Surface enhanced Raman scattering sensing using a coffee-ring-type 3D silver nanostructure self-assembled on glass substrates. **A. Yamaguchi**, T. Fukuoka, R. Hara, Y. Utsumi

20:30 – 730. Microfluidic immunoassay with plug-in liquid crystal for optical detection of antibody. **K. Yang***, Q. Zhu

20:45 – 731. Electrochemical microdevice for the measurement of neutrophil activity for stress monitoring. **M. Yokokawa**, K. Tanabe, A. Yamagishi, Y. Morimoto, M. Kinoshita, H. Suzuki

Marriott Waikiki Beach
Kona Moku Blrm C

Ultrasensitive Assays for Proteins and Protein Modifications (#287)

Organized by: C. Le, H. Zou, N. Dovichi
Presiding: Z. Liu, M. Ye

19:00 – 732. Engineering DNA strand displacement networks for amplified protein detection. **F. Li***

19:30 – 733. Time-resolved luminescence biosensor for dynamic activity detection of protein acetylation-related enzymes based on DNA-sensitized terbium(III) probes. **Z. Nie***

20:00 – 734. Oxidative modifications and structural changes of redox sensitive proteins. **K. Lee***

20:30 – 735. Artificial antibody materials for high sensitive detection of target proteins. **K. Yang**, S. Li, Y. Chen, **L. Zhang***, Y. Zhang

* Principle Author

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Hawaii Convention Center
Halls I, II, III

Advances in FTIR Microspectroscopy: 3D Tomography to Nanoscale Imaging (#315)

Organized by: K. Gough, M. Martin,
M. Chen
Presiding: K.M. Gough, M.C. Martin

Poster Session
19:00 – 21:00

736. Determination of carbonate ion contents in hydroxalcites by FTIR microspectroscopy. **T. Tanaka***, H. Tamai

Friday Morning

Hawaii Convention Center
Halls I, II, III

New Tools and Methodologies for the Characterization of Biomolecular Interactions (#145)

Organized by: S. Krylov, D. Wilson,
W. Zhong, H. Wang
Presiding: S. Krylov, H. Wang

Poster Session
10:00 – 12:00

737. Development of auto-injection system to single cells. **T. Takami***, M. Saito, H. Matsuoka, S. Tate

738. Functional classification method of base materials by interaction analysis with Stratum Corneum. **S. Arai***, M. Iwasa, H. Yoshida

739. Improved DNA equilibrium binding affinity determinations of platinum(II) complexes using synchrotron radiation circular dichroism. **D.L. Ang***, N. Jones, F. Stootman, B. Ghadriani, J. Aldrich-Wright

740. Optical nanoantenna for bacterial detection. **M. Fukuda**, T. Kinoshita, H. Shiggi*, T. Nagaoka

741. Analysis of neuronal cell with atomic force microscopy. **I. Park***, H. Koo, Y. Kim, J. Kim, J. Park

742. Activity of cytoprotective enzymes and apoptosis induced by photodynamic therapy. **C. Jones***

743. Surface enzyme chemistries for single nanoparticle biosensing using surface plasmon resonance microscopy.

A.M. Maley*, H.M. Fung, R.M. Corn

744. Evaluation of peptide-material interaction by force mapping method with an atomic force microscope. **M. Mochizuki**, M. Oguchi, S. Kim, T. Ogawa, G. Lkhamsuren, N. Cho*, T. Hayashi*

745. Kinetic study of intermolecular interaction by capillary electrophoresis: Clathration reaction of thymol with sulfated- β -cyclodextrin. **Y. Shimazaki**, K. Miyabe*

746. Analysis of aggregation-prone regions in monoclonal antibody by hydrogen/deuterium exchange mass spectrometry. **N. Hashii***, S. Nakazawa, M. Tada, Yamaguchi

747. Surface plasmon resonance and fluorescence: A novel approach for characterization of biomolecules interactions.

J. Labrecque-Carbonneau*, J. Masson

748. Electrochemical oxidation: A research tool for drug metabolites with short lives in vivo. **K. Tahara***, Y. Abe, T. Mizushima

749. Early detection of anti-asparaginase to significantly increase remission rate in acute lymphoblastic leukemia therapy. **A. Aubé***, D. Charbonneau, J. Pellerier, J. Masson

750. On-chip templated biosynthesis of unnatural and natural protein microarrays suitable for surface plasmon resonance imaging. **G. Manuel***, R.M. Corn

751. Immobilization of DNA and RNA on QCM sensors modified with self-assembled monolayer of thiol derivatives.

S. Shiba

752. Desired alteration of protein affinities using competitive screening system.

M. Kaishima*, N. Fukuda, J. Ishii, A. Kondo

753. Surface plasmon resonance spectroscopy and nanoplasmonic metal particles for studying biomolecular interactions.

X. Su*

754. Identification of Ryukyu lacquer-wares by pyrolysis-GC/MS and $^{87}\text{Sr}/^{86}\text{Sr}$ isotope ratio measurement. **M. Tetsuo***

755. Structures, stability, and hydrogen bonding in inositol conformers.

N. Siddiqui*

756. Beyond nucleic acids: PCR-based analytics for glycoproteomics and serology.

P. Robinson*

757. Design and synthesis of a novel chemical crosslinker for protein structure determination. **K.M. Downey**, T.L. Pukala

758. Identification and structural analysis of proteins adsorbed from serum to self-assembled monolayers: Components comprising ECM, structural changes, and relevance to cell behavior. Y. Mizushita, T. Nyu, T. Sekine, **T. Hayashi**

759. Siderophore spatial distribution evaluation by direct mass spectrometry imaging on agar Streptomyces cultures.

C.F. Angelini, M.N. Eberlin

760. Time-resolved circular dichroism study on the photodynamics of cyclodextrin encapsulated aromatic molecules.

M. Kuronuma, Y. Araki, S. SAKAMOTO, T. Wada*

761. Nanoparticles-free fluorescence anisotropy amplification assay for detection of RNA nucleotide-cleaving DNase activity. **D. Zhang**, Q. Zhao, H. Wang*

Marriott Waikiki Beach
Milo III

Development and Applications of Techniques for Electrochemical Analysis (#24)

Organized by: J. Chen, D. Arrigan, C. Hu, B. Liu, K. Maeda

8:00 – 762. Electrochemical imaging of cells and tissues. **H.H. Girault***

8:40 – 763. Electrochemical behaviors of NaCl solid-solution microcrystals.

D. Zhan*, D. Huang, Y. Zhu, L. Geng, Z. Tian

9:00 – 764. Probing the surface electrochemical activity of complex natural mineral samples with a microelectrode.

L.A. Jones*, R. Ram, S. Bhargava

9:20 – 765. Light activated electrochemistry: A strategy for performing voltammetry on a monolithic surface where you want, when you want, with micron scale spatial resolution. M.H. Choudhury, S. Ciampi, L. Zarei, R. Tavallaei, V. Goncalves, J. Gooding

9:40 – 766. Electrochemical reduction of RE ions (RE=Dy, Nd, Pr) with Ni electrodes in LiCl-KCl eutectic melts. **H. Konishi***, T. Oishi, T. NOHIRA, H. ONO, E. TAKEUCHI

10:00 Break

10:15 – 767. Synthesis and electrochemical characterization of nanostructured transition metal oxy-hydroxides for supercapacitors of the asymmetric design.

C. Hu*, C. Hsu, K. Chang, H. Hsu

10:35 – 768. Effects of incorporating nanomaterials for the detection of phenolic compounds. **Y. Huang**, **M. Wang***

10:55 – 769. Synthesis and characterization of nanoparticles, thin films, and fibres by the pyrolysis of asphaltenes. **K. Xu**, C. Ayranci, M. McDermott*

11:15 – 770. Voltammetric detection of ozone dissolved in water at a macro boron-doped diamond electrode.

T. Nishiumi*, K.J. Aoki, J. Chen

Marriott Waikiki Beach
Waikiki Bldrm II

Direct and Mediated Bioelectrocatalysis for Biosensors and Energy Conversion Applications (#89)

Organized by: S. Minteer, L. Mao, J. Kim
Presiding: S. Minteer, S. Minteer

8:00 – 771. Engineering the small laccase (SLAC) from *Streptomyces coelicolor* for incorporation into enzymatic biofuel cell cathodes.

K. Garcia, S. Babanova, W. Sheffler, D. Baker, P. Atanassov, **S. Banta***

8:40 – 772. Designing hybrid organic-bio-catalytic reaction cascades. **I. Wheeldon**

9:20 – 773. Spectroelectrochemical analyses of the electron transfer subunit of direct electron transfer type FAD dependent glucose dehydrogenase. **N. Hirose**, N. Suzuki, M. Narita, Y. Yamashita, W. Tsugawa, J. Okuda, K. Kojima, K. Sode*

9:40 Break

10:00 – 774. Paper-based high power enzymatic biofuel cell arrays for self-powered biosensors. **I. Shitanda***, S. Nohara, M. Momiyama, S. Tsujimura, Y. Hoshi, M. Itagaki

10:20 – 775. From mitochondria to metabolons: Enzyme cascade-based bioelectrocatalysis.

S. Minteer, F. Wu, S. Xu

11:00 – 776. Electrosprayed carbon nanofiber supports for photoelectrodes. D. Do*, C. Gumeci, **S. Calabrese Barton**

11:20 – 777. Organic skin patch with built-in enzymatic battery. **M. Nishizawa***

Hawaii Convention Center
Halls I, II, III

Micro- and Nano-fabricated Analytical Devices for Chemical, Biochemical and Biomedical Platforms (#129)

Organized by: Y. Baba, H. Crabtree, S. Jacobson, J. Ramsey, K. Otsuka, D. Chung

Poster Session

10:00 – 12:00

778. Evaluation of the kinetic performance of micro-fabricated 3D structures for LC columns. **M. Nakamura***, T. Naito, T. Kubo, K. Otsuka

779. Microfluidic perfusion culture for vascular biology. **K. Sato***

780. MicroRNA detection on a probe DNA immobilized polymer-grafted surface of the power-free microchip toward point-of-care cancer diagnosis. **R. ISHIHARA**, Y. UCHINO, K. HOSOKAWA, M. Maeda, A. Kikuchi*

781. Passive and continuous hydrodynamic sorting of $\text{PM}_{2.5}$ using a micropost array.

S. Inagaki, T. Yasui, N. Kaji, Y. Baba

782. Development of surface modification and patterning method in extended nanochannels using fluorinated phosphonic acid (FPS)-immobilized TiO_2 . **S. Ishihara**, K. Morikawa, T. Tsukahara*

783. Live cell imaging with quantum dot anti-CD5 antibody conjugates introduced by endocytic pathway. **H. Ueda**, T. Kurabayashi, T. Fukuda*, M. Suzuki

784. Optofluidic devices implemented 3D gold nanostructure enabling surface enhance Raman scattering.

A. Yamaguchi*, T. Fukuda, R. Takahashi, Y. Utsumi

785. Investigation of lipid properties of lanthanoid solutions confined in extended nanospaces. **K. Morikawa**, T. Tsukahara*

786. Development of a dual-function micro-analytical device for DNA separation and label-free detection.

T. Ajiri, T. Yasui, A. Ishida, H. Tani, Y. Baba, M. Tokeshi

787. Titanium oxide-based peptide chip with removal ability of non-specific adsorbant.

S. Nagatomo, K. Yamamoto, S. Matsushima, Y. Katayama, T. Sonoda

788. Microfluidic image-processing-based multipoint crystallization analysis.

A. Akiyama, M. Fukuyama, A. Hibara*

789. Unique properties of water induced by surface chemical groups in extended nanospace.

K. Ikeda, Y. Kazoe, T. Tsukahara, K. Mawatari, T. Kitamori*

790. Structural analysis of water in extended-nano space.

H. Koreeda, K. Mawatari, K. Shiriji, T. Yamaguchi, K. Yoshida, T. Kitamori*

791. Electrical and optical characteristics of gold nanoparticles-deposited microbeads.

Y. Takai, M. Terabe, H. Shiggi*, T. Nagaoka

792. Up-regulation of adipose derived stem cells based on 3D culture using micro-fabricated surface.

K. Yoshimoto

793. Half-integer diffraction background-free optical detection.

K. Furukawa, M. Fukuyama, A. Hibara*

794. Lipid panel test on the disk platform.

C. Shin*, C. Liu

795. Enzyme-linked immunosorbent assay on a disk platform using multistep aliquoting techniques.

H. Wu, C. Shin*, C. Li

796. Selective separation of carbohydrates by capillary gel electrophoresis with PEG-based hydrogels.

H. Furuta, T. Naito, T. Kubo, K. Otsuka

797. Nano-composite with a thermoresponsive molecularly imprinted polymer and a magnetic nanoparticle for selective drug-releasing.

K. Koterasawa*, T. Naito, T. Kubo, K. Otsuka

798. Development of an electrochemical sensor for simultaneous measurement of blood ATP and lactate levels for evaluation of illness severity.

K. Nishiyama, A. Ishida*, H. Tani, M. Tokeshi

799. Invader assay-assisted ELISA for the sensitive detection of disease biomarkers with the naked eye.

Q. Song, Y. Li

800. Microfluidic southern hybridization using microbeads fixed with a photo-cross-linkable resin.

G. Suzuki, K. Tsunoda, K. Sato

801. Retention properties of a C_{60} -fullerene coated silica monolithic capillary in liquid chromatography.

M. Tsuzuki*, Y. Murakami, T. Naito, T. Kubo, K. Otsuka

802. Microflow impulsion and diffusion generated concentration gradient for cell-based assay.

X. Li, L. LIU, J. SHI, F. Zhang, J. HU, L. Wang, z. ZHAO, Y. CHEN*

803. Simple method for the preparation of high diffraction quality protein crystals using microfluidic device.

M. Maeki*, A. Pawate, M. Sugishima, K. Watanabe, M. Tokeshi, P. Kenis, M. Miyazaki

804. High resolution TIRF Imaging of biointerface using self-assembled metal nanoparticle films.

S. Masuda, Y. Yanase, E. Usukura, S. Ryuzaki, K. Okamoto, K. TAMADA*

805. Development of protein concentration system based on pore-size control of molecular sieving gel by thermal-stimulus response.

Y. Fukushima*, T. Naito, T. Kubo, K. Otsuka

806. On-chip metabolism model based on microfluidic technologies for pharmacokinetic study.

H. Kimura*, N. Horio, Y. Sakai, T. Fujii

807. Establishment of analytical method by micro-ELISA for small amount of patient blood.

E. Mori*, A. Yoshizaki, Y. Imai, Y. Hosoya, T. Kitamori*

808. Development of high sensitivity electrode for glucose biosensing system modified by RF magnetron sputtering.

K. Tsuchiya*, J. Tanno, H. Kimura

809. Fundamental studies on controlling sample focusing using nano-micro structures.

Y. Yoshida*, T. Naito, T. Kubo, K. Otsuka

810. Detecting structural variations caused by DNA methylation at the single molecule level in nanochannel.

X. Sun*, T. Yasui, R. Sakon, T. Yanagida, N. Kaji, M. Kanai, K. Nagashima, T. Kawai, Y. Baba

811. Evaluation of a PEG-based hydrogel for protein recognition using molecularly imprinting technique.

S. Arimura*, T. Naito, T. Kubo, K. Otsuka

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S. Arimura*, T. Naito, T. Kubo, K. Otsuka

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S. Arimura*, T. Naito, T. Kubo, K. Otsuka

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S. Arimura*, T. Naito, T. Kubo, K. Otsuka

829. Evaluation of a PEG-based hydrogel for protein recognition using molecularly imprinting technique.

S. Arimura*, T. Naito, T. Kubo, K. Otsuka

830. Evaluation of a PEG-based hydrogel for protein recognition using molecularly imprinting technique.

S. Arimura*, T. Naito, T. Kubo, K. Otsuka

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S. Arimura*, T. Naito, T. Kubo, K. Otsuka

832. Evaluation of a PEG-based hydrogel for protein recognition using molecularly imprinting technique.

S. Arimura*, T. Naito, T. Kubo, K. Otsuka

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S. Arimura*, T. Naito, T. Kubo, K. Otsuka

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S. Arimura*, T. Naito, T. Kubo, K. Otsuka

835. Evaluation of a PEG-based hydrogel for protein recognition using molecularly imprinting technique.

S. Arimura*, T. Naito, T. Kubo, K. Otsuka

836. Evaluation of a PEG-based hydrogel for protein recognition using molecularly imprinting technique.

S. Arim

- 812.** Formation mechanism of lipid nanoparticles in microchannels. **Y. Fujishima**, M. Maeki, T. Yasui, Y. Sato, A. Ishida, H. Tani, H. Harashima, Y. Baba, M. Tokeshi*
- 813.** Automatic assembly of non-spherical microscale particles using electroosmotic flow in a microfluidic device. **H. Moriyama**, T. Ueda*
- 814.** High-sensitive ionic current sensing system using a microfluidic device. **H. Yasaki**, T. Yasui, T. Yanagida, N. Kaji, M. Kanai, S. RAHONG, K. Nagashima, T. Kawai, Y. Baba*
- 815.** Analysis of in vivo biokinetics of transplanted stem cell using cadmium-free quantum dots. **Y. OGIHARA**, H. YUKAWA, D. Onoshima, T. Kameyama, Y. Hayashi, T. Torimoto, T. Ishikawa, Y. Baba
- 816.** NAIMS: Nanotop ambient ionization mass spectrometry. **Z. Zhou**, J. Lee, R.N. Zare
- 817.** Stem cell based bio-actuated microsystem for a micropump using a thin polymer membrane. **Y. Tanaka***, H. Fujita
- 818.** Molecular crowding-assisted on-bead rolling circle amplification for single DNA molecule counting. **N. Sasaki***, Y. Gunji, K. Sato
- 819.** Anchored nanowires for microRNA extraction from extracellular vesicles in body fluid. **D. TAKESHITA**, T. Yasui, Y. He, T. Yanagida, N. Kaji, R. Sakon, M. Kanai, K. Nagashima, T. Kawai, Y. Baba
- 820.** Fluorescence polarization imaging for analyzing molecular interactions. **O. Wakao***, M. Maeki, A. Ishida, H. Tani, A. Hibara, M. Tokeshi*
- 821.** Manipulation and capture of PEGylated ribonuclease A in an insulator-based dielectrophoresis microdevice towards the design of microbioprocesses. M.A. Mata-Gómez, J. González-Valdez, R. Gallo-Villanueva, S. Martínez-Chapa, **M. Rito-Palomares***
- 822.** Recombinant small antibody design for plasmonic biosensor using camel antibody with affinity for target inorganic material. T. Sujino, H. Nakazawa, K. Tawa, R. Asano, I. Kumagai, **M. Umetsu**
- 823.** Current detection in microfluidic devices for measurement of cell deformability. **M. Sano**, T. Yasui, N. Kaji, Y. Baba
- 824.** Stem cells imaging in the second near-infrared region with the use of fluorescence nanoparticles. **T. Shimada**, H. Yukawa, D. Onoshima, H. Niioka, Y. Hayashi, T. Ishikawa, Y. Baba
- 825.** Microfluidic single cancer cells isolation and analysis device by simple manual operation for cytosecreting of cancer stem cells. **Y. Hattori**, D. Onoshima, H. Yukawa, K. Ishikawa, M. Hori, Y. Baba
- 826.** Transportation imaging of exosomes derived from stem cells and cancer cells. **A. Yokoyama**, H. Yukawa, D. Onoshima, Y. Hayashi, T. Ishikawa, Y. Baba
- 827.** Multimodal imaging of stem cells by using quantum and magnetic nanohybrid particles. **R. Naruse**, H. Yukawa, D. Onoshima, Y. Hayashi, T. Ishikawa, Y. Baba
- 828.** Massively parallel detection system of single cells to analyze genomic heterogeneity of cancer cells. **S. Ito**, T. Yasui, N. Kaji, Y. Baba
- 829.** Open-microhole array device with superhydrophilic glass surface for filtering and counting rare tumor cells. **A. Yonese**, D. Onoshima, H. Yukawa, K. Ishikawa, M. Hori, Y. Baba
- 830.** Development of magnetized zinc oxide nanowires by using magnetic fluid. **T. Okawa**, T. Yasui, N. Kaji, Y. He, T. Yanagida, M. Kanai, K. Nagashima, T. Kawai, Y. Baba
- 831.** Development of an observation platform for bacterial activity using conducting polymer films doped with bacteria. **S. Suekuni**, T. Tamura, H. Shigii*, T. Nagaoaka
- 832.** Nanowire devices for analysis of cell-cell communication via extracellular vesicles. **K. Tabuchi***, T. Yasui, Y. He, T. Yanagida, N. Kaji, M. Kanai, K. Nagashima, T. Kawai, Y. Baba

- 833.** High-throughput methylation mapping by detecting fluorescently stained methylation sites at a single molecule level. **A. Hattori**, T. Yasui, N. Kaji, Y. Baba*

Marriott Waikiki Beach
Kona Moku Blrnr B

Optical Waveguide Techniques for the Analyses of Materials and Interfaces (#164)

Organized by: N. Matsuda, S. MENDES, K. TSUNODA, Z. Qi, L. SUN, P. Tassel

8:00 Opening Remarks

- 8:10 – 834.** Integrated bimodal waveguide interferometers for advanced diagnostics. **L.M. Lechuga***

- 8:40 – 835.** Waveguide-based biosensors for the diagnosis of infectious diseases. **h. Mukundan***

- 9:10 – 836.** In situ ATR-IR spectroscopic observations of biointerfaces using a flow cell. **S. Morita***

- 9:40 – 837.** Optical waveguide spectroscopy for study of biological events inside inorganic nanopores. **A. Yamaguchi**

10:10 Break

- 10:30 – 838.** Evaluation of thin film deposition and vapor sorption using optical waveguide spectroscopy with surface plasmon resonance. **K. Shinbo**,

- M. Ishigooka, Y. Ohdaira, A. Baba, K. Kato, F. Kaneko

- 11:00 – 839.** Detection of lead and mercury using silicon-nanowire ring-resonators coated with mesoporous silicates. **H. Look***, S. Borjan, X. Wu, C. Crudden, D. Xu

- 11:30 – 840.** Whispering gallery resonators: New uses in sensing and material analysis. **R. Dunn***, S. Wildgen, D. kim

Marriott Waikiki Beach
Waikiki Blrnr III

Laser Ionization Mass Spectrometry (#274)

Organized by: T. Imaoka, R. Zare, K. Lin
Presiding: R.J. Levis, R.N. Zare

8:00 Opening Remark

- 8:05 – 841.** Laser desorption/ionization droplet delivery mass spectrometry (LDID-MS). **J. Lee**, H. Nam, **R.N. Zare***

- 8:35 – 842.** Application of laser ionization time-of-flight mass spectrometry to emulsion analysis. **H. FUKAYA***, Y. SHIMO*, Y. TSUDA*, H. Ishigami*, **T. UCHIMURA***

- 8:55 – 843.** Nanoparticle seed-layer for laser desorption/ionization mass spectrometry in the quantification of various polarity drugs. **M. Tseng***, R. Obena, Y. Ho, Y. Luo, C. Lin, M. Fu***, Y. Chen**

- 9:15 – 844.** Laser desorption ionization of stilbenes in porous coordination networks. **K. Ohara***, A. Nakai, K. Yamaguchi

- 9:35 Break**

- 9:45 – 845.** MALDI ionization mechanism. **C. Ni**

- 10:15 – 846.** Determination of nerve agent metabolites by gas chromatography/multiphoton ionization/time-of-flight mass spectrometry. **A. Hamachi**, T. Imaoka, Y. Mori, D. Vu, Y. Kida, T. Imaoka

- 10:35 – 847.** Resonant laser mass spectrometry in cultural heritage analysis. **M.S. de Vries***

- 10:55 – 848.** Analysis of pyrolysis products from TiO₂ nanoparticles treated with phenyltriethoxysilane using laser ionization time-of-flight mass spectrometry. **T. Fujii***, **T. UCHIMURA***

- 11:15 – 849.** Ambient femtosecond laser vaporization electrospray ionization mass spectrometry, a universal analysis method. **R.J. Levis**

11:50 Discussion and Conclusion Remarks

Marriott Waikiki Beach
Waikiki Blrnr I

Vibrational Spectroscopy: New Developments and Applications in Biological and Medical Sciences (#375)

Organized by: M. Blades, H. Sato, B. Wood

Presiding: M. Blades, H. Sato, B.R. Wood

Hawaii Convention Center
Halls I, II, III

Ultrasensitive Assays for Proteins and Protein Modifications (#287)

Organized by: C. Le, H. Zou, N. Dovichi

Poster Session

10:00 – 12:00

- 8:50.** Conversion of individual molecules of β -galactosidase between different active conformations using short periods of heating. **D. Craig***

- 851.** Phosphorylation-mediated assembly of semisynthetic fluorescent protein for label-free detection of protein kinase activity. **Y. Huang***, Z. Nie

- 852.** Nanoreactor for large-scale characterization of membrane proteins. **X. Fang**, L. Qiao, B. Liu

- 853.** Application of the fluorescence at 800 nm derived from the interaction with non-fluorescent Cu(II)-porphine to determine human serum albumin. T. Ikeda, H. Sagawa, Y. Nakano, M. Inoguchi, J. ODO

- 854.** Construction of an electroactive peptide probe for sensing of a protein and a cell. **K. Sugawara***, H. Kuramitz, H. Shinohara, T. Kadoya

- 855.** Enhanced Raman spectroscopic immunoassay using an optical interference mirror slide. **M. Yasuda***, T. Akimoto, Y. Ozaki

Marriott Waikiki Beach
Kona Moku Blrnr C

Harmonized Strategy of New UHPLC Implementation in Pharmaceutical R & D and CRO/CMO QC Laboratories (#353)

Organized by: N. Wu, W. Mullett, E. Gong
Presiding: E. Gong, W. Mullett , N. Wu

8:00 Introduction

- 8:10 – 856.** Small-scale ultrahigh performance capillary liquid chromatograph. **M.L. Lee***, S. Sharma, A. Plistil, H.E. Barnett, S.D. Stearns, P.B. Farnsworth, H. Tolley

- 8:40 – 857.** Introduction to UPLC: Theory and practical implementation. **r. Ladd**, **D. Diehl***

- 9:10 – 858.** Evaluation, adoption, and benefits of UPLC at AstraZeneca Pharmaceuticals. **r. Ladd***

- 9:40 – 859.** Pharmaceutical separations using ultrahigh pressure liquid chromatography. **Y.S. Xiang**, M.D. Trone

10:00 Break

- 10:10 – 860.** Applications of UPLC-MS based metabolomics in precision medicine. **G. Xu**, X. Zhao, Z. Yang, P. Yin, X. Lu

- 10:30 – 861.** Application of UHPLC and SPP columns with MS and fusion software for fast and robust method development. **D. Kou***

- 10:50 – 862.** Method transfer from HPLC to UHPLC: Rules, benefits, applications, and eventual problems. **D. Guillarme***, J. VEUTHEY

- 11:10 – 863.** UHPLC vs. HPLC for rapid compound quality control analysis and characterization. **B. Lin***

- 11:30 – 864.** UPLC/UHPLC applications and method transfer in contract research organization (CRO). **W. Huang***, K. Zhou, E. Gong

11:50 Discussion and Conclusion Remarks

Marriott Waikiki Beach
Waikiki Blrnr I

Vibrational Spectroscopy: New Developments and Applications in Biological and Medical Sciences (#375)

Organized by: M. Blades, H. Sato,

B. Wood

Presiding: M. Blades, H. Sato, B.R. Wood

- 8:00 – 865.** Developing clinical diagnostics with deep Raman spectroscopy: Advancing our understanding of spatial distributions of tissue Raman signals. **N. Stone***, M. Vardaki, B. Gardner, P. Matousek

- 8:30 – 866.** Transforming in vitro vibrational spectroscopy into *in vivo* vibrational imaging for applications in biology and medicine. **J. Cheng***, D. Zhang, J. Li, P. Wang

- 8:90 – 867.** Pre-clinical trial on the application of ATR spectroscopy for malaria diagnosis. **B.R. Wood**, J. Heraud, D. Guaita-Perez, P. Jeearanaikoon, P. Tippayawat, D. McNaughton

- 9:20 – 868.** Understanding physiological changes in tissue *in vivo* using Raman spectroscopy. **A. Mahadevan-Jansen***, C. O'Brien, I. Pence, J.C. Slaughter, J.J. Reese, K.A. Bennett

- 9:40 – 869.** Raman spectroscopy for live cells and tissues. **H. Sato**, K. Moor, P. Meksiarun, M. Ishigaki, Y. Maeda

- 10:00 – 870.** Visualising stem cell differentiation status by Raman microspectroscopy. **L. Chiu***, T. Ichimura, K. Fujita, T. Ozawa, H. Fujita*

- 10:20 – 871.** Raman study for monitoring the development of neuronal cell *in vitro*. **K. Hashimoto**, S.N. Kudoh, H. Sato

- 10:40 – 872.** Raman spectral dynamics of single cells in the early stages of differentiation and proliferation upon growth factor stimulation. **S. TAKANEZAWA**, Y. Ozaki, Y. Sako

- 11:00 – 873.** Rapid *in vivo* Raman spectroscopy for early cancer detection – technology development and clinical applications. **H. Zeng***, J. Zhao, M. Short, D. McLean, S. Lam, H. Pawlik, A. McWilliams, H. Liu

- 11:30 – 874.** Bio-Raman spectroscopy as a powerful tool for pathological research and clinical diagnosis. **J. Hu***

Marriott Waikiki Beach
Kona Moku Blrnr A

Advances in Terahertz Spectroscopy and Imaging (#413)

Organized by: A. Rahman, C. Kim, W. Jaeger, S. Nguang
Presiding: A. Rahman, Y. Shamash

8:00 Introduction

- 8:05 – 875.** High resolution spectroscopy with backward wave oscillators. **W. Jaeger***

- 8:35 – 876.** Terahertz characterization of permeation of gold nanoparticles through human stratum corneum *in vitro*. **J. Grove, A. Rahman, T. Ramezanli, B. Michnai-Kohn, A. Rahman***

- 9:05 – 877.** In vitro study of the non-thermal effect of terahertz-wave irradiation. **N. Yaekashiwa**, S. Hayashi, K. Kawase

- 9:25 – 878.** Terahertz pulsed spectroscopy of paraffin-embedded brain glioma. **j. li, k. meng, T. Chen, L. Zhu, Z. Li**

9:45 BREAK

- 10:00 – 879.** Early detection of skin cancer by terahertz reflectometry, spectroscopy, and imaging. **B. Rao***, A. Rahman, A. Rahman*

- 10:30 – 880.** Role of human sweat duct in terahertz wave interaction with human skin. **S.R. Tripathi***, E. Miyata, K. Kawase

* Principle Author

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<http://pacificchem.org/onlineprogram>

10:50 – 881. Self-association and intermolecular vibrations of dimethyl sulfoxide in cyclohexane solutions studied by THz TDS, mid-IRS, and DFT calculations.
K. Mizuno

11:10 – 882. Monitoring hydrogen bonds in soft materials by terahertz spectroscopy.
H. Hoshina, H. Suzuki, S. Yamamoto, S. Yajima, Y. Ozaki, C. Otani

11:30 – 883. Even technology entrepreneurs need partners: what it takes in today's world.
Y. Shamash

Friday Afternoon

Marriott Waikiki Beach
Milo III

Development and Applications of Techniques for Electrochemical Analysis (#24)

Organized by: J. Chen, D. Arrigan, C. Hu, B. Liu, K. Maeda

13:00 – 884. Generator-collector effects in electroanalytical processes.
F. Marken*

13:30 – 885. Metal nanoparticle-attached nickel electrodes for electroanalysis.
M. Oyama*

13:50 – 886. Novel electrochemical analysis of hydrophilic and lipophilic natiocidants in bicontinuous microemulsion.
E. Kuraya, D. Kato, O. Niwa, M. Kunitake

14:10 – 887. Direct and indirect molybdenum enzyme electrochemistry.
P.V. Bernhardt*

14:30 – 888. Photoelectrochemical immunoassays.
H. Chen*

14:50 Break

15:00 – 889. Nanogap sensors.
L. Rassaei

15:20 – 890. Bioanalysis and metabolism strategy based on electrochemistry and mass spectrometry.
B. Liu*, X. Fang, L. Qiao, X. Zhang, H.H. Girault

15:40 – 891. Diffusive relaxation hinders the time response of electrochemical detection in microchannels.
R. Trouillon*, M.A. Gijis

16:00 – 892. Development of a reconfirmable DNA sensing protocol on polycrystalline silicon nanowire field effect transistor.
Y. Yang*

16:20 – 893. Electrochemical studies of protein kinase catalyzed phosphorylations.
H. Kraatz

16:40 – 894. Insight into electrochemiluminescence of Au25 clusters.
Z. Ding

17:00 Closing Remarks

Marriott Waikiki Beach
Waikiki Blrm II

Direct and Mediated Bioelectrocatalysis for Biosensors and Energy Conversion Applications (#89)

Organized by: S. Minteer, L. Mao, J. Kim
Presiding: S. Minteer, S. Minteer

13:00 – 895. Direct electron transfer of glucose oxidase at seamless 3D graphene-carbon nanotubes hybrid for glucose sensing and biofuel cell.
A. Mulchandani*, T. Terse-Thakoor, K. Komori, P. Ramnani

13:40 – 896. Nanobiocatalytic approaches for improving both lifetime and electron transfer rate of bioelectrocatalysis.
J. Kim

14:20 – 897. Direct extracellular electron transfer via noncovalent flavin cofactor in outer membrane cytochrome of *Shewanella* and *Geobacter* species.
Y. Tokunou, K. Hashimoto*, A. Okamoto*

14:40 – 898. Directed biomolecule immobilization on comb-branched DNA.
E.K. TeSelle*, D.A. Baum

15:00 – 899. Human biosensing by micro-electrode double potential pulse.
J. Burgess*

15:40 – 900. Novel first generation enzymatic biosensors via spontaneous adsorption of enzymes on nitrogen-doped carbon nanotubes.
K.J. Stevenson*, J. Goran, I. Rust

16:20 – 901. Non-faradaic unlabeled electrochemical capacitive detection of DNA modification and hybridization process using custom-made gold interdigitated microelectrode arrays.
N.E. Solis Marcano*, M. Lopez-Nieves, C.R. Cabrera

16:40 – 902. Employing DNA for bioelectrocatalysis.
D.A. Baum

Marriott Waikiki Beach
Milo IV / V

Novel Analytical Probes for In Vivo Optical Functional Imaging (#115)

Organized by: Y. Urano, T. Ozawa, Y. Chang, M. McCarroll
Presiding: T. Ozawa

13:00 – 903. Optical imaging and analysis of cell-death pathways using bioluminescent proteins.
T. Ozawa

13:25 – 904. Genetically-encoded luminescent indicator applicable in millisecond voltage phenomena.
T. Nagai*

13:50 – 905. Live cell imaging and in vivo analysis for temporal reaction of G protein-coupled receptor using split luciferase complementation.
M. Hattori, T. Ozawa*

14:10 – 906. Video rate imaging of local tensors for structural characterization of collagen by second harmonic generation microscopy.
G.J. Simpson*

14:30 – 907. Fluorescent probe for single-molecule live-cell imaging of telomeric repeat containing RNA using fluorescent protein reconstitution and an RNA-binding domain PUM-HD.
H. Yoshimura, T. Yamada, H. Segawa, T. Ozawa*

14:50 Break

15:05 – 908. Improvement of two-photon microscopy using a new optical technology.
T. Nemoto*

15:30 – 909. Raman tags: Nonfluorescent chemical probes for small molecules.
K. Fujita*

15:55 – 910. Study on intracellular SERS and multispectral imaging.
A. Shen*, J. Hu

16:15 – 911. 3D layered neuronal networks constructed in biomimetic scaffolds.
M. Yoon*

Marriott Waikiki Beach
Kona Moku Blrm B

Optical Waveguide Techniques for the Analyses of Materials and Interfaces (#164)

Organized by: N. Matsuda, S. MENDES, K. TSUNODA, Z. Qi, L. SUN, P. Tassel

13:00 – 912. Wideband integrated photonics for chemical detection at surfaces.
J.S. Wilkinson*, G.S. Murugan

13:30 – 913. Ex situ waveguide spectroscopy technique for characterization of ultrathin solid-state films.
Z. Qi*

14:00 – 914. Surface plasmon-waveguide coupled emission for probing thick samples up to micrometer-scale.
Y. Li*, Q. Liu, S. Cao, S. Huo, K. Xie, Y. Zhai, Y. Weng

14:30 – 915. Optimal structures and various applications of a waveguide-mode sensor.
M. Fujimaki*

15:00 Break

15:20 – 916. Introduction to optical waveguide multi-platform development and fundamental applications.
H. Takahashi*

15:50 – 917. Dye adsorption in mesoporous silica film characterized by polarized optical waveguide spectroscopy.
D. Lu*

16:10 – 918. Optical fiber total internal reflection fluorescence with a liquid core waveguide for collecting/delivering fluorescence photons.
S. Tao*, C.A. Guyer

16:30 – 919. Planar waveguide ATR and TIRF spectroscopy in the time- and frequency-domains: Development and application to photochemical and electrochemical reactions in molecular films.
S. Saavedra*

Marriott Waikiki Beach
Waikiki Blrm III

Laser Ionization Mass Spectrometry (#274)

Organized by: T. Iimasaka, R. Zare, K. Lin
Presiding: C. Ni, R. Zimmerman

13:00 – 920. Combustion, crude oil, coffee roasting, and industrial processes: Analysis of complex materials and thermal processes by photo-ionisation mass spectrometry (PIMS).
R. Zimmerman

13:30 – 921. Application of tunable vacuum-ultraviolet (VUV) light coupled with reflectron time-of-flight mass spectrometry for the isomer-specific detection of complex organic molecules in astrophysical ice analogs.
M.J. Abplanalp, R. Kaiser

13:50 – 922. Unraveling the gas-phase chemistry in chemical vapor deposition with cyclic organosilicon precursors using laser ionization mass spectrometry.
Y. Shi*, I. Badran, L. Tong

14:10 – 923. Time-of-flight mass spectrometry of polycyclic aromatic hydrocarbons and their analogs.
Y. Tang, T. Iimasaka, S. Yamamoto, T. Iimasaka

14:30 Break

14:40 – 924. Some applications of laser-based ionization mass spectrometer in molecular photodissociation.
K. Lin

15:10 – 925. Mechanical study of reaction pathways in solid nitromethane (CH_3NO_2) and D3-nitromethane (CD_3NO_2) upon interaction with ionizing radiation.
P. Makasyuk*, M. Förstel, R. Kaiser

15:30 – 926. Characterization of thermal decomposition products of chemical vapor deposition precursors using vacuum ultraviolet photoionization time-of-flight mass spectrometry.
J. Zhang*

15:50 – 927. Online monitoring of the dispersed oil of an emulsion using laser ionization mass spectrometry.
Y. TSUDA*, T. UCHIMURA*

16:10 – 928. Femtosecond ionization in mass spectrometry for observing a molecular ion.
T. Iimasaka*

16:35 Closing Remark

Marriott Waikiki Beach
Milo I

Advanced Analytical Applications and Technical Developments of Soft X-Ray Spectroscopy (#303)

Organized by: Y. Muramatsu, S. Hayakawa, C. Heske, A. Buuren, A. Moewes
Presiding: S. Hayakawa, Y. Muramatsu

13:00 Opening Remarks

13:05 – 929. Conversion electron yield XAFS measurements with soft X-rays for element selective measure of specific surface area.
S. Hayakawa, E. Tsuji

13:25 – 930. Characterization of contact lens polymer gels: Cryo vs. dried methodology.
D. Kapur*

13:45 – 931. N-K absorption spectra of small cluster structures in a hydrated biocell.
T. Ejima, M. Kado, M. Aoyama, K. Yasuda, S. Tamotsu

14:05 – 932. Chemical imaging of atmospheric aerosols.
M.K. Gilles, S.T. Kelly, B. Wang, A. Laskin

14:25 – 933. Novel system to study the element-specific valence electronic structure of wet materials.
Y. Harada

15:05 – 934. PPM detection limits in powder X-ray diffraction guided by second harmonic generation imaging.
G.J. Simpson*

15:25 – 935. Quasi in situ XPS analysis on hydrocarbon decomposition on a TiO_2 surface by UV irradiation.
N. Ohtsu*

15:45 – 936. Characterization on blue apatite beads recovered from Tell el-Kerkh, Syria (pottery Neolithic period) and related materials.
C. NUMAKO, K. Kitahara, Y. Shimazu, Y. Taniguchi

16:05 – 937. Soft X-ray absorption absorption/reflectivity analyses of carbon materials in BL10 at the NewSUBARU.
Y. Muramatsu*, T. Uemura, K. Nambu, D. Fukuyama, M. Kuki, T. Harada, T. Watanabe, H. Kinoshita

16:25 Break

16:40 – 938. Probing the ground state oxygen holes and the metal-insulator transition in strained rare earth nickelate films with Resonant Inelastic X-ray Scattering.
T. Schmitt*

Marriott Waikiki Beach
Waikiki Blrm I

Vibrational Spectroscopy: New Developments and Applications in Biological and Medical Sciences (#375)

Organized by: M. Blades, H. Sato, B. Wood
Presiding: M. Blades, H. Sato, B.R. Wood

13:00 – 939. Surface-enhanced Raman spectroscopy: From biomolecules to live-cell imaging.
B. Ren*, X. Zheng, L. Xu, C. Zong, M. Xu, J. Zhang

13:30 – 940. Gold nanoparticles as a substrate in bio-analytical near-infrared surface-enhanced Raman spectroscopy.
H.J. Butler*, S. Fogarty, F.L. Martin

14:00 – 941. Molecular and elemental imaging approaches to investigate the relationship between vitamin B12 and multiple sclerotic lesions in human brain tissue.
P. Heraud, S. Petratous, P. Doble, B.R. Wood

14:20 – 942. Developmental stages in the directed differentiation of human pancreatic insulin-positive cells characterized using Raman microspectroscopy.
M. Blades, T. Kieffer, R. Turner, J. Piret, S. Konorov, H. Schulze, B. Gage

14:40 – 943. Separation of Raman and fluorescence signals by wavelength modulation with parallel accumulation.
R. Shimada, T. Nakamura, T. Ozawa*

15:00 – 944. Development of a highly-sensitive time-resolved IR spectrometer and its application to high-background aqueous biological samples.
M. Kubo*, T. Kimura, Y. Yamaguchi, S. YANAGISAWA, R. Komiya, J. Yan, S. Nakashima, T. OGURA, Y. Shiro

15:20 – 945. Tip-enhanced Raman spectroscopy of biomaterials.
F. Pashaei, M. Tabatabaei, F. Lagugné-Labarthet*

15:40 – 946. Plasmonic nanopipettes toward cell secretion monitoring by dynamic SERS.
F. Lussier*, J. Masson

16:00 – 947. Analysis of urine metabolites by sheath-flow SERS detection.
Z.D. Schultz*

16:20 – 948. Study of mouse embryo by Raman spectroscopy.
M. Ishigaki*, K. Hashimoto, N. Ogawa, K. Morimoto, Y. Ozaki, H. Sato

16:40 – 949. Raman monitoring of anticancer drug effect in live mouse model.
A. Taketani, B.B. Andriana, H. Sato

* Principle Author

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Marriott Waikiki Beach
Kona Moku Blrm A

Advances in Terahertz Spectroscopy and Imaging (#413)

Organized by: A. Rahman, C. Kim, W. Jaeger, S. Nguang
Presiding: W. Jaeger, J. Uddin

13:00 Introduction

13:05 – 950. Interaction of TiO_2 nanoparticles with human dermal cells via terahertz scanning reflectometry.

A. Rahman*, T. Mironava, A. Rahman, M. Rafailovich

13:35 – 951. Time-resolved THz spectroscopy and its application to 1D/2D materials. J. Park*, W. Lee, H. Choi, T. Kim, S. Jung, J. Bae, M. Cho*

13:55 – 952. Terahertz investigation of nanostructured TiO_2 enhanced natural dye sensitized solar cell. J. Uddin*, A.D. Ward, N.N. Brown, A. Rahman, A. Rahman

14:25 – 953. Investigating the low frequency vibrations of jet-cooled biomolecules with chirped-pulse THz spectroscopy. E.G. Buchanan, D.F. Plusquellec*

14:45 BREAK

15:00 – 954. Sub-surface corrosion detection by terahertz time-domain reflection spectrometry and 3D imaging.

D. Hadzilalic*, A. Rahman

15:30 – 955. Terahertz sub-surface scanning and 3D imaging for semiconductor wafer defect detection. A. Rahman, A. Rahman*

15:50 – 956. Ultrafast terahertz modulation characteristics of photo-induced metal-insulator transition of W-doped VO_2 film. Z. Zhai*, Y. Xiao, L. Zhu, W. Huang

16:10 – 957. Crystal structure and thermal behavior of low molecular weight poly(3-hydroxybutyrate) studied by terahertz and Raman spectroscopy. T. Miyai*, N. Kadoya, H. Hoshina, Y. Ozaki, H. Sato

16:30 – 958. Terahertz spectroscopic polarimetry of archimedean spiral arrays: Experiments and simulations.

C. Schmuttenmaer, D.J. Aschaffenburg, M.R. Williams

16:50 Closing remarks

Friday Evening

Hawaii Convention Center
Halls I, II, III

Optical Waveguide Techniques for the Analyses of Materials and Interfaces (#164)

Organized by: N. Matsuda, S. MENDES, K. TSUNODA, Z. Qi, L. SUN, P. Tassel

Poster Session

19:00 – 21:00

959. UV-visible spectral analysis of azobenzene crystals with optical waveguide spectrometer. T. Taniguchi, M. Shiro, H. Koshiba*, T. ASAHI

960. Speciation analysis for aluminum with a liquid-core/liquid-cladding optical waveguide. S. Yoshizawa*, H. Murata, K. Sato, K. Tsunoda

961. Nucleobase-functionalized conjugated polymer for detection of copper(II).

C. Xing, H. Yuan, Y. Zhan

Marriott Waikiki Beach
Kona Moku Blrm C

Ultrasensitive Assays for Proteins and Protein Modifications (#287)

Organized by: C. Le, H. Zou, N. Dovichi
Presiding: Z. Nie, L. Zhang

19:00 – 962. Targeting cancer biomarkers by molecularly imprinted polymers. Z. Liu*

19:30 – 963. Enhancing the sensitivity of MS-based proteomics and phosphoproteomics using TrEnDi. K. Wasslen, K. Blank, Z. Naperstkov, S. Shields, J.M. Manthorpe*, J.C. Smith*

20:00 – 964. Peptide N-terminal protection strategy for deep glycoproteome analysis. M. Ye*, J. Huang, Z. Zhang, K. Cheng, F. Wang, H. Zou*

20:30 – 965. Multiplexing microfluidics reactor for integrated proteolysis. L. Yan, J. Ji, B. Liu, P. Yang

Hawaii Convention Center
Halls I, II, III

Advanced Analytical Applications and Technical Developments of Soft X-Ray Spectroscopy (#303)

Organized by: Y. Muramatsu, S. Hayakawa, C. Heske, A. Buuren, A. Moewes
Presiding: Y. Muramatsu

Poster Session
19:00 – 21:00

966. Preparation and characterization of boron/carbon thin film having diamond-like structure. T. Kimoto*, M. Kawaguchi, N. Ohno, H. Enomoto, Y. Muramatsu

967. Study on the sorption behavior of Pt and Pt complex anions onto $\delta\text{-MnO}_2$. K. Tanaka*, D. Kawamoto, H. Ohashi, M. Tokunaga, Y. Okae, T. Yokoyama

968. Chemical state of gold supported on catalyst precursor. H. Ando*, D. Kawamoto, H. Ohashi, Y. Okae, M. Tokunaga, T. Yokoyama

969. Development of in-situ battery cell for X-ray absorption spectroscopy.

R. Miyahara*, M. Katayama, Y. Inada

970. Identification of edge-carbon atoms in hexagonal carbon layers by C K-XANES measurements of nanographite particles and theoretical assignments using the first-principle calculations. T. Okada, Y. Muramatsu, K. Murayama

971. Application of soft X-ray spectroscopy to characterization of nitrogen ion implanted TiO_2 photocatalysts.

T. Yoshida*, S. Niimi, M. Yamamoto, S. Ogawa, T. Nomoto, S. Yagi

972. Evaluation of the weathered Japanese roof tiles of the Himeji Castle by soft X-ray absorption spectroscopy. Y. Muramatsu*, R. Murakami

Hawaii Convention Center
Halls I, II, III

Vibrational Spectroscopy: New Developments and Applications in Biological and Medical Sciences (#375)

Organized by: M. Blades, H. Sato, B. Wood

Presiding: M. Blades, H. Sato, B.R. Wood

Poster Session
19:00 – 21:00

973. Study of protein secondary structure by using NIR and Raman spectroscopy.

K. MORIMOTO, M. Ishigaki, Y. Ozaki

974. Studies performed at the beamline for infrared microspectroscopy at the MAX IV laboratory in Lund Sweden. A. Engdahl

975. Correlation between hydrophilic lipophile balance number and percutaneous permeation of optically active amino acid ions into horny intercellular fat of skin.

Y. WATANABE*, N. HIGASHI, T. UEDA, K. SHIOYA, M. MATSUMOTO, H. SUZUKI

976. Raman spectroscopy-observed a single colorectal adenocarcinoma in living animal. B.B. Andriana, A. Taketani, H. Sato

977. Estimation of body fat amount of a laboratory mouse by using Near-Infrared spectrometer. N. Ogawa*, K. Fujiwara, Y. Sato, K. Okada

978. Development and application of infrared scattering-type near-field scanning optical microscopy. H. Kwon*, E. Lee

979. Novel DNA electrophoresis analysis using near-infrared spectroscopy.

M. Yasuda*, T. Akimoto, Y. Ozaki

980. Investigation of the interaction between biomimetic membranes and protein aggregates using various spectroscopic techniques. R. Karaballi*, C.L. Brosseau

981. Use of attenuated total reflectance Fourier transform infrared spectroscopy to monitor surface tethered phospholipids via copper-free click chemistry.

E.N. Towns, D.P. Land*

982. Structural monitoring in DOPC and DynePC in nanolipoprotein particles resulting from polymerization as determined by attenuated total reflectance Fourier transform infrared spectroscopy.

J. Moore*, S. Gilmore, E.N. Towns, H. Guo, C. Blanchette, D.P. Land

983. High-resolution Raman imaging of lipid rafts in artificial monolayer membranes.

J. Ando, M. Kinoshita, J. Cui, H. Yamakoshi, K. Dodo, K. Fujita, M. Murata*, M. Sodeoka*

984. Raman spectroscopic study on the spore formation process of fission yeast at starvation state.

T. Yamamoto*, T. Sasaki, H. Noothapati, T. Kaino, M. Kawamukai, H. Hamaguchi

985. In situ surface-enhanced Raman spectroelectrochemistry of a hemin modified nanostructured gold surface.

E. Carlen, L. Le Thi Ngoc

986. Thin layer chromatography/coupling reaction-based surface enhanced Raman scattering for a facile detection of carbofuran.

T. Sukmanee, K. Wongravee, S. Ekgasit, C. Thammacharoen, P. Pinepinjitham*

987. Living cell analysis on the effect of endocrine disruptor by Raman spectroscopy.

N. Ogawa, K. Hashimoto, A. Oguro, S. Imaoka, H. Sato

988. Analysis of human pancreatic cancer cell line by confocal Raman spectroscopy.

M.E. Jan, S.S. Alzahrani, B.B. Andriana, H. Sato

Hawaii Convention Center
Halls I, II, III

Advances in Terahertz Spectroscopy and Imaging (#413)

Organized by: A. Rahman, C. Kim, W. Jaeger, S. Nguang

Presiding: W. Jaeger, M. Rafailovich, A. Rahman, J. Uddin

Poster Session

19:00 – 21:00

989. Development of wide dynamic range terahertz-wave spectrometer based on optical parametric process in lithium niobate crystal.

K. Imayama*, K. Murate, S. Hayashi, H. Minamide, K. Kawase

990. Single shot measurement of terahertz pulses based on pulse front tilting by reflective grating.

Z. Zhai*, S. Zhong, L. Zhu

991. Recognition of chemicals concealed under covering substances using terahertz spectroscopy based on injection-seeded terahertz parametric source.

M. Kato*, R. Yamazaki, K. Murate, K. Imayama, K. Kawase

992. Optical characterization of hydrogen-bonded materials at terahertz frequencies.

K. Takeya*, R. Takahashi, K. Kawase

993. High power and broadband terahertz wave generation from $LiNbO_3$ ridge waveguide.

T. Minami, H. Okano, K. Takeya, K. Kawase

994. Isothermal crystallization of poly glycolic acid(PGA) by terahertz and Infrared spectroscopy.

F. Nishimura*, Y. Ozaki, H. Hoshina, H. Sato

Saturday Morning

Hawaii Convention Center

Halls I, II, III

Development and Applications of Techniques for Electrochemical Analysis (#24)

Organized by: J. Chen, D. Arrigan, C. Hu, B. Liu, K. Maeda

Poster Session

10:00 – 12:00

995. Mechanism of controlling oil droplet contact angle through three-phase boundary reaction.

Y. Yang, K.J. Aoki, J. Chen

996. Variables of solvents controlling electric double layer capacitance at highly oriented pyrolytic graphite.

Z. Wang, K.J. Aoki, J. Chen*

997. Structural analysis of $Li_4Ti_5O_{12}(111)$ surfaces in ionic liquid by frequency modulation atomic force microscopy.

T. Uchida*, M. Kitta, T. Ichii,

T. Utsunomiya, H. Sugimura

998. Localized electrochemical deposition property analysis by image feedback and simulation.

y. ciou*, Y. Ren, L. Jing Chie,

, Yao-Tien

999. Cobalt phthalocyanine/nitrogen-doped graphene nanocomposite for electro-analysis of thiols.

H. Xu*, B. Liu*

1000. Measurements of single ion activity of hydrogen ion in concentrated aqueous electrolyte solutions using the ionic liquid salt bridge.

R. Hashimoto*, R. Nakamura, M. Yamamoto, T. Kakiuchi,

R. Murakami

1001. Determination of the single ion activity of hydrogen ion in sulfuric acid solutions measured by us of ionic liquid salt bridge.

R. Nakamura*, R. Hashimoto,

M. Yamamoto, T. Kakiuchi, R. Murakami

1002. Applying the electrochemistry of simple redox systems (quinones and phenylenediamines) for comparisons of the hydrogen bond strengths of alcohols in organic solvents.

M.E. Tessensohn,

R.D. Webster*

1003. Electrochemical evaluation of bacterial viability using fluorescent labels.

M. Takai, K. Ishiki, H. Shigui*, T. Nagaoka

1004. Detection of electrocatalytic activity of individual nanoparticle using microelectrochemical device.

J. Joo*, S.J. Kwon

1005. Observation of different current responses by electrocatalytic amplification of platinum single nanoparticle collision on silver ultramicroelectrodes.

S. Mun*, S.J. Kwon

1006. Effect of solution pH on the corrosion resistance and characterization of the composite film formed on Mg alloy by steam coating.

N. Kamiyama*, T. Ishizaki

1007. Verification of the geometric constant K for electrochemical time of flight experiments.

J.C. Moldenhauer*, M. Meier,

D. Paul

1008. Impact of different grinding aid on standard deviation in x ray fluorescence analysis of cement raw meal.

A. Tyopine*

1009. Photoinduced electron transfer reaction of C_60 at a nitrobenzene/water interface.

M. Fujimori*, T. Hinoue

1010. Ion-transfer voltammetry of streptothricin antibiotics with differently sized lysine oligomers at a nitrobenzene/water interface.

K. Uematsu*, C. Maruyama,

Y. Hamano, H. Katano

1011. Gold oxide formation and stripping voltammetry for water analysis in room temperature ionic liquids.

J.C. Aguilar*, A. García Mendoza

1012. Ion voltammetric determination of alkali metal ions with a flow electrolytic cell.

R. Nakamura*, T. Hinoue

1013. Electrochemical analysis of Cu(II) complexes in copper sulfate electropolating solution as compared with colorimetric analysis by using reaction kinetics with a chelate reagent.

H. Noma*, T. Koga,

K. Nonaka

1014. General strategy for photoelectrochemical immunoassay using an enzyme label combined with a CdS quantum dot/TiO₂ nanoparticle composite electrode.

W. Zhao*, J. Xu, H. Chen

* Principle Author

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- 1015.** Application of the voltammetric reduction using a strong alkaline electrolyte to corroded copper plate samples exposed in air at East Asian countries, Japan, Korea, and Taiwan. **T. Ozeki***, S. Fujiwara, S. Nakayama, T. Osakai
1016. Characterization of fluorine substituted LiFeBO₃ as a cathode material for lithium rechargeable battery. **J. An**, J. Bak, H. Lee, Y. Lee*

Marriott Waikiki Beach
Waikiki Blrm II

Direct and Mediated Bioelectrocatalysis for Biosensors and Energy Conversion Applications (#89)

Organized by: S. Minteer, L. Mao, J. Kim
Presiding: S. Minteer, S. Minteer

- 8:00 – 1017.** Biomolecular studies of the intra- and intermolecular electron transfer in the FAD dependent dehydrogenase complex capable of direct electron transfer. **K. Sode**

- 8:40 – 1018.** On the role of flavins in bacterial extracellular electron transfer via outer membrane cytochromes: Closer, molecular perspective. **S. Babanova**, I. Matanovic, P. Atanassov

- 9:20 – 1019.** Application and immobilization of a novel naphthoquinone derivative for mediated bioelectrocatalysis of glucose by FAD-dependent glucose dehydrogenase. **R.D. Milton**, S. Minteer*, D. Hickey, S. Abdellaoui, K. Lim, B. Tan

- 9:40 – 1020.** Iron-sulfur cluster is conserved in the catalytic subunits of direct electron transfer type FAD dependent dehydrogenase complexes. **M. Shioya***, K. Kojima, W. Tsugawa, T. YAMAZAKI, S. Ferri, K. Sode*

- 10:00 – 1021.** Enzymatic, microbial, or abiotic cathodic catalysis in bioelectrochemical systems (BECS). **C. Santoro***, A. Serov, K. Artyushkova, S. Babanova, P. Atanassov

- 10:20 – 1022.** Robust microbial ureolysis self-sustaining system for the removal of urea from urine. **M. Morales**, R. Martinez, R. Morales, I. González-González, C.R. Cabrera

- 10:40 – 1023.** Direct and mediated multi-enzyme sensor for continuous glucose and lactate monitoring. **E. Takagi**, A. Suzuki, S. Tsujimura, K. Kojima, W. Tsugawa, K. Sode*

- 11:00 – 1024.** Direct bioelectrocatalysis of PQQ-dependent pyranose dehydrogenase adsorbed on a glassy carbon electrode at various pH levels. **K. Takeda**, H. Matsumura, T. Ishida, M. Yoshida, K. Igarashi, M. Samejima, N. NAKAMURA*, H. Ohno

- 11:20 – 1025.** Engineering of glucose oxidase after electron acceptor preferences in the oxidative half reaction.

C. Maeda, S. Saito, Y. Horaguchi,

S. Vogt, G. Nöll, K. Sode*

- 11:40 – 1026.** Disentangling the extracellular electron transfer mechanisms of *She-wanella oneidensis* MR-1 on graphite and indium tin oxide electrode. **S. Xu**, M.Y. El-Naggar*

Marriott Waikiki Beach
Milo IV / V

Novel Analytical Probes for In Vivo Optical Functional Imaging (#115)

Organized by: Y. Urano, T. Ozawa, Y. Chang, M. McCarroll
Presiding: Y. Urano

- 8:00 – 1027.** Chemical mechanism of selective cytotoxicity induced by silica-phthalocyanine-based near infrared photoimmunotherapy. **H. Kobayashi***

- 8:25 – 1028.** Porphysome nanotechnology for in vivo optical imaging and beyond. **G. Zheng**

- 8:50 – 1029.** Development of novel fluorogenic probes for peptidases and glycosidases and their application to rapid intraoperative imaging of tiny tumors. **Y. Urano***

- 9:15 – 1030.** Fluorescence-guided digestive surgery using indocyanine green and novel fluorescence prove activated by pancreatic chymotrypsin. **T. Ishizawa**, Y. Urano, M. Kamiya, S. Yamashita, N. Kokudo, A. Saura

9:40 Break

- 9:55 – 1031.** Imaging tumor cells using uptake of fluorescent L-glucose derivatives. **K. Yamada***

- 10:20 – 1032.** Development of in vivo imaging probes for vulnerable plaque detection. **M. Ogawa***, K. Shimizu, Y. Narita, M. Maess, Y. Magata, N. Oku

- 10:45 – 1033.** Novel strategy for deeply penetrating photoacoustic cancer imaging. **M. Ishihara***, T. Teranishi, Y. Urano

- 11:10 – 1034.** Switching of near-infrared absorption and generation of reactive oxygen species via diradical complexes for cancer theranostics. **K. Tamura***, A. Masuya, N. Iki

Marriott Waikiki Beach
Kona Moku Blrm A

Marine and Freshwater Toxins: Detection, Structure, and Pharmacology (#138)

Organized by: T. Tsumuraya, J. Hungerford, R. Lewis
Presiding: T. Tsumuraya

8:00 Introductory Remarks

- 8:05 – 1035.** World of benthic dinoflagellates viewed by chemistry. **T. Yasumoto***

- 8:45 – 1036.** Accelerated detection of ciguatoxins using LC/MS and functional bioassays. **R.J. Lewis***

- 9:25 – 1037.** Detection of ciguatoxins from marine creatures caught off Japanese waters by LC-MS. **N. Oshiro**

10:05 Break

- 10:20 – 1038.** Absolute quantification of ciguatoxins standard by quantitative nuclear magnetic resonance. **T. Kato**, N. Sugimoto, K. Ishizuki, T. Suematsu, M. Nagae, S. Inohara, K. Fujita, M. Watai, T. Yasumoto*

- 10:40 – 1039.** Algal toxins: Development of analytical and bioassay detection methods and assessment of environmental transfer in marine food webs. **P. Lam***, L. Chan, Y. MAK, J. Wu, T. Wai

- 11:20 – 1040.** Detection of sodium channel toxins using both viability and membrane depolarization endpoints. **R. Manger***, D. Woodle, A. Berger, C. Greene, J. Hungerford

Marriott Waikiki Beach
Waikiki Blrm I

Optical Waveguide Techniques for the Analyses of Materials and Interfaces (#164)

Organized by: N. Matsuda, S. MENDES, K. TSUNODA, Z. QI, L. SUN, P. Tassel

- 8:00 – 1041.** Waveguide evanescent field fluorescence (WEFF) and waveguide evanescent field scattering (WEFS) microscopy. **S. Mittler***

- 8:30 – 1042.** In situ observation of direct electron transfer reaction of cytochrome c immobilized on ITO electrode modified with 10-carboxydecylphosphonic acid. **N. MATSUDA***, H. Okabe

- 9:00 – 1043.** Developments of liquid-core/liquid-cladding optical waveguides for liquid/liquid interface studies. **K. TSUNODA***, Y. Hasegawa, S. Yoshizawa, K. Sato

- 9:30 – 1044.** Label-free high resolution surface plasmon microscopy for quantitative cell-gold interface investigation. **K. Toma***, H. Kano, A. Offenbässer

10:00 Break

- 10:20 – 1045.** In situ observation of adsorption-desorption process and direct electron transfer reaction between cytochrome c and ITO electrode modified with self-assembled monolayer films. **H. Kawazumi***, S. Ikeda, H. Okabe, N. MATSUDA

- 10:40 – 1046.** Electrochemical characterization of redox processes using single-mode electro-active integrated optical waveguides. **X. Han**, S.B. Mendes

- 11:10 – 1047.** Critical importance of gap modes in surface enhanced Raman scattering. **M. Futamata***, M. Ishikura, C. Iida, K. Arai

Marriott Waikiki Beach
Milo I

Advanced Analytical Applications and Technical Developments of Soft X-Ray Spectroscopy (#303)

Organized by: Y. Muramatsu, S. Hayakawa, C. Heske, A. Buuren, A. Moewes

Presiding: C. Heske, A. Moewes

- 8:00 – 1048.** Ordered structure of Fe-N-containing carbonaceous thin film characterized by soft X-ray spectroscopy. **J. Maruyama**, T. Amano, Y. Domi, T. Doi, Y. Muramatsu

- 8:20 – 1049.** Characterization of carbon doping on chemical states of amorphous Ge₂Si₂Te₅, measured with high-resolution X-ray photoelectron spectroscopy. **Y. Lee**

- 8:40 – 1050.** Effect of molecular order on the carbon near edge X-ray absorption fine structure (NEXAFS) spectra of poly(3-hexyl-thiophene). **M. Martinson**, S. Eger, B. Collins, H. Ade, **S. Urquhart**

- 9:00 – 1051.** Operando soft X-ray spectroscopic analysis of chemical potential shift in organic field-effect transistors. **N. Nagamura***, Y. Kitada, J. Tsurumi, H. Matsui, K. Horiba, I. Honma, J. Takeya, M. Ohshima

- 9:20 – 1052.** Characterization of a hydrolytic precipitate of [AuCl₄]⁻ complex ion. **D. Kawamoto***, H. Ohashi, Y. Okae, S. Utsunomiya, M. Tokunaga, T. Yokoyama

9:40 Break

- 10:00 – 1053.** About the bandgap of 2D materials graphene and silicene. **A. Moewes***, A. Hunt, N. Johnson, D. Muir

- 10:40 – 1054.** O 1s X-ray photoelectron spectra (1486 eV to 5000 eV) of bulk *n*-conductor Na-silicate glasses and vitreous SiO₂: Oxygen speciation and minimum linewidths. **Y. Hu**, Q. Xiao, D. Wang, X. Cui, H. Nesbitt, **G. Bancroft**

- 11:00 – 1055.** Electronic and chemical structure of GaInP₂ thin films for photoelectrochemical water splitting studied by soft X-ray spectroscopies. **M. Blum***, J.L. Young, D.A. Duncan, S.G. Rosenberg, H. Dörscher, F. Meyer, A. Benkert, R.G. Wilks, M. Bär, L. Weinhardt, W. Yang, T. Deutsch, J.A. Turner, C. Heske

Marriott Waikiki Beach
Kona Moku Blrm B

Bacterial Identification by Mass Spectrometry (#389)

Organized by: K. Voorhees, J. Banoub, K. Teramoto

- 8:00** Opening remarks, Kent J. Voorhees

- 8:00 – 1056.** Rapid characterization of microorganisms by mass spectrometry: An overview. **C. Fenselau***

- 8:35 – 1057.** Metal oxide laser ionization (MOLI) MS for identification of bacteria using fatty acid profiling. **K.J. Voorhees***, N.R. Saichel, R.A. Jensen, C.R. McAlpin, C.R. Cox

- 9:00 – 1058.** Strain-level fungal identification by CeO₂-catalyzed MALDI-TOF MS fatty acid analysis. **C.R. Cox***, K.J. Voorhees

- 9:25 – 1059.** Qualitative and quantitative detection of bacteria in complex human matrices using taxon-specific markers. **N. Strittmatter***, J. McKenzie, A.V. Speller, A. Burke, P. Pruski, R. Mirnezami, J. Marchesi, M. Rebec, Z. Takats

- 9:50 – 1060.** eMALDI: boosting quantitative MALDI by electrowetting-supported sample preparation. **O. Kudina, B. Eral, F. Mugele**

10:15 Break

- 10:25 – 1061.** Cystic fibrosis microbial ecology of a human lung. **N. Garg***, E. Hyde, A. Bouslimani, J. Wu, R. Wong, G. Lin, D. Conrad, T. Alexandrov, R. Knight, P. Dorrestein

- 10:50 – 1062.** Bacterial discrimination by proteotyping based upon the S10-GERMS method. **H. Tamura***

- 11:25 – 1063.** Rapid top-down proteomic identification of Shiga toxin 2 subtypes from pathogenic *Escherichia coli* using MALDI-TOF-TOF-MS/MS and post-source decay. **C.K. Fagerquist***, W.J. Zaragoza

Marriott Waikiki Beach
Milo III

Organized Surfactant Assemblies in Chemical Analysis and Separation Science: Fifty Years Later (#457)

Organized by: W. Hinze, T. Saitoh, G. Jiang, J. Liu
Presiding: W. Hinze, T. Saitoh

8:00 Opening Remarks - WL Hinze

- 8:05 – 1064.** Micelles in separation science: From small molecules to proteins to nanoparticles. **R. Nagarajan**

- 8:35 – 1065.** Surfactant-mediated separation for efficient wastewater treatment. **T. Saitoh***

- 9:15 – 1066.** State of the art in micellar liquid chromatography. **A. Berthod***

- 9:55 – 1067.** Surfactants and micelles in separations and mass spectrometry: Looking back and looking forward. **D.W. Armstrong***

- 10:35 – 1068.** MEKC in 30 years. **K. Otsuka***

- 11:15 – 1069.** Modeling the effects of micelles and micelle-like organized systems on reactivity and equilibria, with implications in analytical chemistry. **F. Quina***

Saturday Afternoon

Marriott Waikiki Beach
Waikiki Blrm II

Comprehensive Multidimensional Separations (#90)

Organized by: T. Gorecki, F. Dorman, P. Haddad
Presiding: F. Dorman, T. Gorecki

- 13:00 – 1070.** Introduction to comprehensive multidimensional separation. **T. Gorecki***

- 13:20 – 1071.** Applications of planar microfluidic devices and gas chromatography for complex problem solving. **R.A. Shellie**

- 13:40 – 1072.** Concept of (low-)flow modulation comprehensive 2D gas chromatography under sub-ambient, ambient, and supra-ambient pressure outlet conditions. **L. Mondello***

* Principle Author

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14:00 – 1073. Q-TOF mass spectrometer coupled with GCxGC using atmospheric pressure chemical ionization: Toward a universal mass spectrometry-based system for environmental analysis.

K. Jobst*, L. Haimovici, X. Ortiz, M. Robson, D. Megson, S. Fernando, A. Lada, D. Stevens, G. O'Sullivan, P. Helm, E. Reiner

14:20 – 1074. 2D comprehensive gas chromatography multireflection high resolution time-of-flight mass spectrometry: Merging accurate mass information with multidimensional chromatographic resolution. **R. Zimmermann**, T. Gröger, B. Wegler

14:40 – 1075. Comprehensive 2D gas chromatography with chiral columns in both dimensions to study enantioselective interconversion processes. **P.J. Marriott**, S. Kroeger , Y. Wong

15:00 – 1076. Power of comprehensive 2D gas chromatography for target and non-target compound analysis. **J. Cochran***, F. Dorman, M. Misselwitz, M. Merrick

15:20 – 1077. Vacuum-UV detection for GC: Why all the buzz? **J.J. Harynuk***, B.M. Weber, L.A. Adutwum, K.A. Stevenson

15:40 – 1078. CEMS: Consensus estimation of multidimensional shift, a new tool for aligning GCxGC chromatograms.

S. Furbo*, G. Tomasi, J.H. Christensen

16:00 – 1079. Improvements to thermodynamic-based predictions of GC and GCxGC separations. **K.A. Stevenson**, H. Ebrahimi-Najafabadi, J. Harynuk

16:20 – 1080. Predicting the properties of petroleum with pixel-based analysis of GCxGC data. **S. Furbo***, A.B. Hansen, R.G. Egeberg, J.H. Christensen

16:40 – 1081. Recent advances in the use of GCxGC-(HR)TOFMS for the characterization of complex VOC mixtures of biological interest. **J. Focant***, P. Stefanuto

Marriott Waikiki Beach
Milo IV / V

Novel Analytical Probes for In Vivo Optical Functional Imaging (#115)

Organized by: Y. Urano, T. Ozawa, Y. Chang, M. McCarroll

Presiding: Y. Chang

13:00 – 1082. Universal imaging probe development for almost everything.

Y. Chang

13:25 – 1083. Development of pancreatic β -cell probe and its application for in vivo imaging. **N. Kang**, J. Lee, S. Park, W. Phue, B. Agrawall, A. Firdaus

13:50 – 1084. Intracellular and in vivo oxygen sensing using phosphorescent iridium (III) complexes. **S. Tobita***, T. Yoshihara, M. Hosaka, T. Takeuchi

14:15 – 1085. Two-photon time-resolved emission imaging microscopy in microsecond domain: From FLIM to PLIM with transition metal complexes. E. Baggaley, S. Botchway, I.V. Sazanovich, J. Haycock, J. Williams, **J.A. Weinstein***

14:35 Break

14:50 – 1086. Two-photon uncaging of photo-TOF releasers and vasodilation in living mouse brain. **H. Nakagawa**

15:15 – 1087. Toward in vivo manipulation of intracellular signaling pathways.

T. Furuta

15:40 – 1088. Functional fluorescence probe for lipid derived radicals detection.

K. Yamada*

16:00 – 1089. Detection of lacZ-positive cells in living tissue with single-cell resolution. **M. Kamiya**, T. Doura, Y. Urano

16:20 – 1090. Development of a series of NIR dark quenchers based on Si-rhodamines and their application to fluorescence probes. **K. Hanaoka**, T. Myochin, Y. Urano*

Marriott Waikiki Beach
Kona Moku Blrrm A

Marine and Freshwater Toxins: Detection, Structure, and Pharmacology (#138)

Organized by: T. Tsumuraya, J. Hungerford, R. Lewis
Presiding: J. Hungerford

13:00 Introductory Remarks

13:05 – 1091. Practical route to the left wing of CTX1B and synthesis of haptien-KLH conjugate: Total syntheses of CTX1B and 54-deoxyCTX1B. **S. Yamashita***, K. Takeuchi, T. Koyama, T. Tsumuraya, M. Inoue, I. Fujii, M. Hirama

13:40 – 1092. Sandwich ELISA detection of ciguatoxins using anticiguatoxin monoclonal antibodies. **T. Tsumuraya***

14:15 – 1093. Near real time detection of ciguatoxins using a field-portable surface plasmon resonance sensor system.

S.D. Soelberg, T. Tsumuraya, M. Hirama, T. Yasumoto, I. Fujii, **C.E. Furlong***

14:50 Break

15:05 – 1094. Toxicokinetics of Pacific ciguatoxins (P-CTXs) in orange-spotted groupers (*Epinephelus coeruleopunctatus*). **Y. MAK**, Y. Kang, J. Wu, P. Lam, Y. Chen, L. Chan*

15:25 – 1095. Detection and structure elucidation of marine toxins by several LC/MS techniques. **T. Suzuki***, D. Viet Ha, A. Uesugi, H. Uchida, R. Matsushima, R. Watanabe, H. Nagai, M. Kamio, M. Adachi

16:00 – 1096. Comparison of ELISA, quantitative MALDI-TOF and LC-MS/MS for the determination of microcystins.

M. Pirez, L. del Puerto, A. Perez-Parada, G. Saona, Gonzalez-Sapienza, **B.M. Brenna***

16:20 – 1097. Role of biomarkers for monitoring brevetoxins in *Karenia brevis* exposed molluscan shellfish. **A. Abraham***, S.M. Plakas

Marriott Waikiki Beach
Waikiki Blrrm III

Paper-Based Analytical Devices for Point of Need Measurements (#213)

Organized by: D. Citterio, C. Henry,
J. Brennan
Presiding: D. Citterio, C. Henry

13:00 Opening Remarks

13:05 – 1098. Quantitative electrochemical detection of analytes at sub-picomolar levels using a simple paper sensor.

R.M. Crooks*, J.C. Cunningham, M. Kogan, P. DeGregory, M. Tsai, X. Li

13:35 – 1099. Development of boron-doped diamond paste microelectrode on paper-based analytical device for simultaneous determination of norepinephrine and serotonin. **S. Nantaphol**, T. Kondo, W. Siamproh, O. Chaiapakul, C. Henry

13:55 – 1100. All-in-one ion-sensing platform based on paper and colloid-imprinted mesoporous carbon. J. Hu, A. Stein, W.H. Smyrl, **P. Buhlmann***

14:15 – 1101. Paper diagnostic device for picomolar level detection of ricin using a galvanic exchange based immunosensing strategy. **J.C. Cunningham**, R.M. Crooks*, M. Kogan, M. Tsai, L. Luo, I. Richards, A. Ellington

14:35 – 1102. Fundamentals of printing flow barriers on filter paper. **R. Pelton**, S. Jahanshahi-Anbuhri, K. Pennings, B. Kannan, J.D. Brennan, C. Filipe

15:05 Break

15:15 – 1103. Inkjet printing of protein and aptamer bioinks for production of bioactive paper sensors. **J.D. Brennan***

15:35 – 1104. Out of the lab and into the world: Chemical analysis with paper millifluidic devices in Kenya, South Africa, and Burkina Faso. N. Myers, A. Weaver, **M. Lieberman***

15:55 – 1105. Reader-free paperfluidic analytical device for fluorescence-based tear lactoferrin detection. **K. Yamada**, T.G. Henares, K. Suzuki, D. Citterio*

16:10 – 1106. Inkjet-printed microfluidic paper-based analytical devices (μ PADs) for colorimetric cation detection.

D. Citterio*, T.G. Henares, S. Takaki, H. Shibata, N. Komuro, K. Yamada, K. Suzuki

16:30 – 1107. Paper-based analytical devices for rapid titrations. **T. Kaneta***

Marriott Waikiki Beach
Milo I

Advanced Analytical Applications and Technical Developments of Soft X-Ray Spectroscopy (#303)

Organized by: Y. Muramatsu, S. Hayakawa, C. Heske, A. Buuren, A. Moewes
Presiding: C. Heske, T. Van Buuren

13:00 – 1108. New insight into the metal-to-insulator transition in vanadium oxide.

K.E. Smith*, J. Laverock, A. Zakharov, S. Kittiwatanakul, S. Wolf, J. Lu

13:40 – 1109. Mercury species in activated carbon with added potassium sulfide or calcium chloride. **M. Takaoka***, A. Sano, K. Shioota, D. Hamaguchi

14:00 – 1110. Adsorption-desorption behavior of trace-level alkali metals on oxides and micaceous oxides. **Y. Baba**, I. Shimoyama, N. Hirota, T. Izumi

14:20 – 1111. Characterization of cadmium cation adsorbed on a surface of silica by XAFS spectroscopy. **H. Ohashi**, H. Ando, K. Tanaka, D. Kawamoto, A. Miyazaki, Y. Okabe, T. Yokoyama

14:40 Closing Remarks

14:45 Break

15:00 Introduction to Special Session for Prof. Dennis Lindle

15:10 – 1112. Synergies between AMO physics and materials science: A tribute to Dennis Lindle. **C.S. Farley***

15:40 – 1113. Photoelectron dynamics in the "tender" X-ray domain: A tribute to Dennis Lindle. **M. Piancastelli***

16:10 Break

16:30 – 1114. Mass spectrometry and resonant inelastic X-ray scattering with tenderness: A tribute to Dennis Lindle. **M. Simon***

17:00 – 1115. Nondipole and interchannel coupling effects in X-ray photoionization: A tribute to Dennis Lindle. **S.T. Manson***

17:30 – 1116. Non-dipole effects in atomic and molecular photoionization in the soft X-ray range and the continuing legacy of Dennis Lindle. **K.P. Bowen***

Marriott Waikiki Beach
Kona Moku Blrrm C

Analytical Laser-Induced Breakdown Spectroscopy (LIBS) for Hazards Analysis, Forensics, and Health (#379)

Organized by: J. Almirall, J. Almirall, Y. Deguchi, A. Miziolek, S. Rehse, Z. Wang
Presiding: Z. Wang

13:00 – 1117. Mars geochemical investigations with ChemCam and SuperCam.

S.M. Clegg*, R.C. Wiens, S. Maurice, O. Gasnault, o. Forni, S.K. Sharma, A.K. Misra, R. Anderson, N. Lanza

13:40 – 1118. Deep-sea laser-induced breakdown spectroscopy. **B. Thornton***, T. Sakka, T. Takahashi, T. Sato, T. Ohki, K. Ohki

14:10 – 1119. Development of laser remote analysis for nuclear fuel materials under severe environments. **I. Wakaida***, K. Akaoka, M. Miyabe, H. Ohba, M. Saeki, C. Ito, M. Oba, M. Kato

14:40 Coffee Break

15:00 – 1120. Laser induced breakdown spectroscopy (LIBS): A potential tool to study impacts of CO_2 leakage on ground water quality. C. Goueguel, C. Carson, H. Sanghani, J. Jain, D. McIntyre*

15:30 – 1121. First Responder and forensic applications of a handheld laser-induced breakdown spectroscopy instrument.

R.R. Hark*, A. Miller, J. Plumer, D. Day

16:00 – 1122. Quantitative analysis of coal using laser induced breakdown spectroscopy. **Z. Wang***, Z. Hou*

Marriott Waikiki Beach
Waikiki Blrrm I

Advances in Analytical Techniques for Effective Food Allergen Management (#394)

Organized by: N. Lee, S. Godefroy, S. Taylor, H. Akiyama, J. Baumert, M. Shoji
Presiding: H. Akiyama, S. Godefroy

13:00 Opening

13:05 – 1123. Food allergen labeling in Japan. **M. Ebisawa***

13:40 – 1124. Consumer perspective on food allergen management. **C. Eldred**

13:55 – 1125. Food allergy prevalence - U.S. **S.L. Taylor**

14:25 – 1126. Japanese framework for labeling and testing of allergens in foods. **H. Akiyama**, R. Adachi

14:55 Break

15:10 – 1127. Method development of food allergen analysis. **M. Shoji***

15:40 – 1128. 2S albumin as a stable marker for allergen residue detection: A case study with a sandwich immunoassay specific to Ara c3 for the detection of cashew nut residues in food. **Y. Zhao**, X. Sun, C. Marquis, **N.A. Lee***

16:10 – 1129. Methods for detecting partially hydrolyzed gluten and soy allergens in food. **L.S. Jackson***

16:40 – 1130. Digestion resistance of macadamia nut proteins and allergenicity of the digested products. **J. Rost**, S. Muralidharan, S.L. Taylor, J. Baumert, N.A. Lee*

Marriott Waikiki Beach
Milo III

Organized Surfactant Assemblies in Chemical Analysis and Separation Science: Fifty Years Later (#457)

Organized by: W. Hinze, T. Saitoh, G. Jiang, J. Liu
Presiding: G. Jiang, J. Liu

13:00 – 1131. Interaction thermoresponsive polymers and surfactants and its application to chemical analysis. **N. Uehara***, M. Mori

13:35 – 1132. Use of surfactants for the separation of nanomaterials in complex matrices. **J. Liu***, R. Liu, J. Chao, S. Yu, X. Zhou

14:15 – 1133. Identification and potential application of emerging quaternary ammonium surfactants in municipal sewage sludge. **T. Ruan**, **G. Jiang**

14:55 – 1134. One-pot preparation of nanoparticle chains via self-assembly of in situ synthesized gold nanoparticles in a zwitterionic surfactant-rich medium.

Y. Takagai*, H. Tran Thi, W. Hinze

15:35 – 1135. Tunable hydrogel for enantioselective drug delivery. **I.M. Warner***, K. McNeel, S. Das, N. Siraj, I. Negulescu

16:15 – 1136. Enantiomeric selectivity of self-assembled guanosine monophosphate in aqueous solution.

L.B. McGown*

* Principle Author

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Saturday Evening

Hawaii Convention Center
Halls I, II, III

Direct and Mediated Bioelectrocatalysis for Biosensors and Energy Conversion Applications (#89)

Organized by: S. Minteer, L. Mao, J. Kim
Presiding: S. Minteer

Poster Session

19:00 – 21:00

1137. Direct electron transfer-type H₂/O₂ biofuel cell with dual-gas-diffusion system. **Q. SONG**, Y. Kitazumi, O. Shirai, K. Kano*

1138. Electrochemical techniques reveal multiple pathways for electron transport in microbial anode respiration. **R. Yoho**, S. Popat, C. Torres*

1139. Direct electron transfer of a PQQ domain of pyranose dehydrogenase on Au electrodes. **R. Kusuoka**, K. Takeda, K. Igarashi, M. Samejima, N. NAKAMURA*, H. Ohno

1140. Electrostatic interaction between enzymes and electrodes in the electric double layer examined in a view of direct electron transfer-type bioelectrocatalysis. **Y. Sugimoto***, Y. Kitazumi, O. Shirai, M. Yamamoto, K. Kano

Hawaii Convention Center
Halls I, II, III

Novel Analytical Probes for In Vivo Optical Functional Imaging (#115)

Organized by: Y. Urano, T. Ozawa, Y. Chang, M. McCarroll
Presiding: Y. Urano

Poster Session

19:00 – 21:00

1141. Asymmetric rhodamine-based fluorescence probes for multicolor in vivo imaging. **R.J. Iwatake**, M. Kamiya, Y. Urano*
1142. Analysis of the fluorescence quenching mechanism of *N*-phenyl rhodamines and its application to a fluorescence probe for HaloTag protein. **S. Iwaki**, K. Hanaoka, K. Yoshida, M. Uchiyama, Y. Urano*

1143. Fluorescence-guided detection of peritoneal metastatic tumors with sensitive β -galactosidase-activatable fluorescence probe. **D. Asanuma***, M. Sakabe, M. Kamiya, K. Yamamoto, J. Hiratake, p. choyke, T. Nagano, H. Kobayashi, Y. Urano*

1144. Lysosomal enzyme-activatable fluorescence probes for specific and sensitive cancer imaging. **K. Yamamoto**, M. Kamiya, Y. Urano

1145. Naphthalene-based zinc chemosensor and its application of bioimaging in HeLa-cell and *Arabidopsis*. **M. Gyuri**, S. Jung, J. Jung*

1146. Protein-conjugated K⁺ probe that detects K⁺ efflux on cell membrane. **T. Terai***, T. Hirata, T. Nagano, Y. Urano*

1147. Construction of a library of asymmetric Si-rhodamine fluorophores and its application to ratiometric fluorescence probes. **Y. Kagami**, K. Hanaoka, T. Nagano, Y. Urano*

1148. Design and synthesis of new caging groups having cell type specificity. **Y. Iketani**, A.Z. Suzuki, T. Furuta*

1149. Latent caged cAMPs that can be photoactivated in the presence of specific enzymes. **T. Sakano**, A.Z. Suzuki, T. Ueno, M. Saitoe, T. Furuta*

1150. Development of various fluorescent sensors based on coumarin scaffold. **T. Shiraishi**, T. Hirano, Y. Noji, T. Saito, H. Kagechika*

1151. Metal-carbonyl clusters as photo-acoustic contrast agents – toward near-infrared in vivo imaging. **Z. Lam**, G. Balasundaram, K. Kong, W. LEONG*, M. Olivo*

1152. Facile protein-directed Co-template synthesis of near-infrared based dual-emission fluorescent nano-hybrid of quantum dots - gold nanoclusters for target-responsive ratiometric bio-imaging in vitro and in vivo. **Z. Nie***

Hawaii Convention Center
Halls I, II, III

Marine and Freshwater Toxins: Detection, Structure, and Pharmacology (#138)

Organized by: T. Tsumuraya, J. Hungerford, R. Lewis
Presiding: J. Hungerford, R.J. Lewis, T. Tsumuraya

Poster Session

19:00 – 21:00

1153. Dynamic distribution and toxic effects of chronic sub-lethal exposure of P-CTX-1 on mice. **J. Wu***, L. Feng*, Y. MAK, P. Lam, L. Chan*

1154. Study of the biosynthesis of paralytic shellfish toxins using stable isotope labeled intermediates and LC-MS. **S. Tsuchiya**, Y. Cho, K. Konoki, K. Nagasawa, Y. Oshima, M. Yotsu-Yamashita*

1155. Sensitive detection of okadaic acid from shellfish samples using a portable surface plasmon resonance (SPR) detection system. **S.D. Soelberg***, K. Campbell, C. Elliott, C.E. Furlong

1156. Simultaneous analysis of saxitoxin analogs and their biosynthetic intermediates by HILIC-LC-MS/MS. **Y. Cho***, R. Yoshioka, S. Tsuchiya, K. Konoki, Y. Oshima, M. Yotsu-Yamashita

1157. New lyngbyatoxin derivatives from the cyanobacterium *Moorea producens*. **W. Jiang**, S. Tan, W. Zhou, H. Uchida, Y. Hanaki, K. Irie, R. Watanabe, T. Suzuki, M. Kamio, H. Nagai*

1158. Accelerated extraction procedure for LC-MS/MS confirmation of Caribbean ciguatoxin in fish. **H.A. Flores Quintana***, C.R. Loeffler

1159. Trends of ciguatera fish poisonings in Japan. **M. Toda**, S. Sakugawa, Y. Nakama, T. Takamine, H. Toyofuku, N. Oshiro*

Hawaii Convention Center
Halls I, II, III

Paper-Based Analytical Devices for Point of Need Measurements (#213)

Organized by: D. Citterio, C. Henry, J. Brennan

Poster Session

19:00 – 21:00

1160. Paper-based fluoroimmunoassay for rapid and sensitive detection of an animal biomarker. **S. Mohammadi**, M. Maeki, A. Ishida, H. Tani, M. Tokeshi*

1161. Microfluidic paper-based analytical devices for analysis of nitrite, uric acid, and pH with a 3D printer for fabrication devices. **H. Asano***, Y. Shiraishi

1162. Clinical enzymology by paper spray mass spectrometry. **X. Yan**, X. Li, C. Zhang, K. Moore, Y. Xu, R.G. Cooks

1163. Parameters influencing the performance of inkjet-printed microfluidic paper-based analytical devices. **R. Ota**, K. Yamada, K. Suzuki, D. Citterio*

1164. Going mobile: Transitioning DE-TECHIP from a 96-well plate test to a printed array with phone app intergration. **R.M. Burks***, A. Holmes, J. Atwater

1165. Determination of Fe(II) in hot spring water using microfluidic paper-based analytical devices. **K. Ogawa**, T. Kaneta*

1166. Microfluidic-paper-based devices for aflatoxin B₁ analysis. **L.A. Busa***, M. Maeki, A. Ishida, H. Tani, M. Tokeshi

1167. Improvement of dipping time of dye nanoparticle-coated test strip for metal ion detection using moisture-retaining agents. **Y. Takahashi**, N. Kanai, S. Souma

1168. Graphene-polyaniline modified electrode for DNA biosensor using paper-based electrochemical device. **P. Teengam***, W. Siangproh, A. Tuantranont, T. Vilaivan, O. Chailapakul

1169. Fabrication and evaluation of screen-printed paper-based three-electrode chip having instantly usable solid-state KCl/Ag/AgCl reference electrode. **M. Komoda***, I. Shitanda, M. Itagaki, Y. Hoshi

1170. Paper test card for quantifying beta-lactam antibiotics. **N. Myers**, D. Aldulaimi, M. Lieberman

1171. Microfluidic paper-based detection system for capillary immunosensing. **K. Kido**, T.G. Henares, K. Suzuki, D. Citterio*

1172. Silk screening using fabric screen ink for rapid mass fabrication of paper-based analytical devices: Application to salivary thiocyanate testing. **J. Sitanurak**, T. Amornsakchai, N. Ratanawimarnwong, D. Nacapricha*

1173. Chelate titrations using microfluidic paper-based analytical devices. **S. Karita**, T. Kaneta*

1174. Development of a point-of-need diagnostic device for detection of myoperoxydase. **M. Wolfe**, P. Nair, J.D. Brennan*

1175. Inkjet-printed paper-based ion optode devices. **H. Shibata**, T.G. Henares, N. Komuro, K. Suzuki, D. Citterio*

1176. Disposable material integrated analytical platforms. **W. Liao***, C. Wang, C. Chen

Hawaii Convention Center
Halls I, II, III

Analytical Laser-Induced Breakdown Spectroscopy (LIBS) for Hazards Analysis, Forensics, and Health (#379)

Organized by: J. Almirall, Y. Deguchi, A. Mizolek, S. Rehse, Z. Wang

Presiding: A. Mizolek

Poster Session

19:00 – 21:00

1177. Applications of laser induced breakdown spectroscopy and laser-breakdown time-of-flight mass spectrometry to conventional boilers, IGFC, and iron and steel making processes. **Y. Deguchi***, F. Shiou, Z. Wang, S. Katsumori, A. Ikutomo

1178. Development of a LIBS-based coal quality analyzer for application to power plant. **L. Zhang**

1179. Methods for quantitative analysis of submerged solids for application to deep-sea LIBS. **T. Takahashi***, B. Thornton, T. Sakka, T. Sato, T. Ohki, K. Ohki

1180. Rapid detection of metallic elements in vegetables by single pulse laser induced breakdown spectroscopy. **M. Yao***

1181. In situ monitoring of additives and wear metals in flowing lubricating oil. **M.J. Dickerson**

1182. Quantitative multi-element analysis of heavy metal ions in an aqueous solution by electrodeposition-assisted underwater laser-induced breakdown spectroscopy. **A. Matsumoto***, A. Tamura, K. Fukami, N. Nishi, K. Amano, T. Takahashi, T. Sato, B. Thornton, T. Sakka

1183. Laser remote isotope analysis for highly-radioactive nuclear fuel materials. **M. Miyabe***, M. Oba, M. Kato, K. Akaoka, I. Wakaida

1184. Reactions of atomic species in laser ablation plasma in water: The cause of rapid decrease in underwater LIBS signals. **T. Sakka***, A. Kawasaki, A. Matsumoto, A. Tamura, T. Honda, K. Amano, N. Nishi

1185. Investigation of local thermal equilibrium in laser-induced plasmas in water: Measurements of atomic excitation temperatures. **T. Honda***, A. Matsumoto, K. Amano, N. Nishi, T. Sakka

1186. Determination of carbon isotopes by laser ablation molecular isotope spectrometry (LAMIS). **J. Jain***, a. Bolshakov, x. Mao, D. McIntyre, R.E. Russo

1187. Application of spatial confinement for gas analysis using laser-induced breakdown spectroscopy to improve signal stability. **Z. Hou**, Z. Wang

1188. Impact of moisture content on coal analysis using laser induced-breakdown spectroscopy. **T. Yuan**, M. Chen, Z. Wang

Hawaii Convention Center
Halls I, II, III

Bacterial Identification by Mass Spectrometry (#389)

Organized by: K. Voorhees, J. Banoub, K. Teramoto

Poster Session

19:00 – 21:00

1189. High-throughput identification of coliforms in processed soybean products using matrix-assisted laser desorption ionization time-of-flight mass spectrometry. **M. Katase***, K. Tsumura

1190. Identification of nontuberculous mycobacteria using matrix-assisted laser desorption/ionization-time of flight mass spectrometry as a rapid diagnostic tool. **I. Hayashi***, M. Onodera, S. Kayama, T. Hara, Y. Koba, M. Yozozaki, H. Ohge, M. Sugai

1191. Contrasting the lipidomes of field-collected vs. lab-cultured organisms: Challenges for lipid-based identification methods. **N.A. Pianegonda***, I. Jamil, T. Huynh, P.J. Barker, S. Blanksby, S.A. Rice, T.W. Mitchell

1192. Rapid identification of histamine-producing bacteria by MALDI-TOF MS. **S. Uehara***, M. Kobayashi, Y. Suzuki, R. Katoh, S. Matsushita, Y. Higuchi, T. Chiba, A. Hirai, A. Kai, K. Sadamasu, K. Kato

1193. Application of Kendrick mass defect plot analysis for identification of mycolic acid-containing bacteria by using high mass-resolution MALDI spiral-TOFMS. **K. Teramoto***, T. Sato, R. Cody, T. Tamura, M. Hamada, H. Komaki, K. Suzuki

1194. Practical applications of MALDI-TOF MS microbial analysis in food and beverage industries. **K. Togami**, H. Ikemoto, R. Ishii

1195. Evaluation of typing methods of *Bacillus coagulans* strains as food spoilage bacteria. **J. Sato**, A. Horiuchi, D. Tomiyama, I. Sonoda, M. Nakayama, M. Hasumi, T. Miyamoto

1196. Biomarkers research involved in salmonid diseases: An approach based on MALDI-MS coupled with data mining techniques. **X.A. López Cortés***, V. Olate, F. Nachtigall, M. Ríos-Monberg, L. S. Santos

1197. Expansion of MALDI-TOF MS database for spoilage microorganisms in food and beverage industry. **K. Togami***, M. Nakayama, J. Sato, I. Kato, S. Maeda, F. Aoyama, N. Takahashi, H. Ikemoto

* Principle Author

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Hawaii Convention Center
Halls I, II, III

Advances in Analytical Techniques for Effective Food Allergen Management (#394)

Organized by: N. Lee, S. Godefroy, S. Taylor, H. Akiyama, J. Baumert, M. Shoji

Presiding: N.A. Lee

Poster Session
19:00 – 21:00

1198. Quantification of sugars in breakfast cereals using capillary electrophoresis. M. Touounji, **M. Van Leeuwen***, J. Oliver, A. Shrestha, M. Gaborieau, P. Castignolles

1199. Developing an optical sensor to detect polyamines and assay enzyme activity of diamine oxidase. **H. Lin**

Hawaii Convention Center
Halls I, II, III

Organized Surfactant Assemblies in Chemical Analysis and Separation Science: Fifty Years Later (#457)

Organized by: W. Hinze, T. Saitoh, G. Jiang, J. Liu

Presiding: W. Hinze, T. Saitoh

Poster Session
19:00 – 21:00

1200. Homogenous liquid-liquid extraction using weak acidic fluorine-based surfactant and its application to separation and recovery method for rare earth elements. **S. Saito***, T. Kato, H. Yamaguchi, S. Igarashi

1201. Cloud point extraction of metallic nanoparticles using zwitterionic surfactants. **A. Endo**, W. Hinze

1202. Approach to the structural analysis of PFOA/TBA⁻ ionic liquid used in homogeneous liquid-liquid extraction method (HoLE). **S. Suzuki***, Y. Takagai, S. Oshita, S. Igarashi

1203. Liposome immunoassay based on bioluminescent detection and its application to on-chip analysis. **Y. Nakatani**, M. Maeki, R. Mishra, D. King, A. Ishida, J. Duerée, M. Tokeshi, H. Tani

Sunday Morning

Marriott Waikiki Beach
Waikiki BlrM II

Comprehensive Multidimensional Separations (#90)

Organized by: T. Gorecki, F. Dorman, P. Haddad

Presiding: T. Gorecki, P.R. Haddad

8:00 – 1204. Pixel-based analysis of the kinetics of petroleum desulfurization. **S. Furbo***, A.B. Hansen, T. Skov, J.H. Christensen

8:20 – 1205. Determination of chlorinated paraffins in surface waters using comprehensive gas chromatography. D. Vassová, P. Oswald, J. Slobozník, **I. Špánik***

8:40 – 1206. Utilizing GCxGC-TOFMS and GCxGC-HRTOFMS to determine the source of a groundwater supply contamination incident due to Marcellus shale gas development. **F. Dorman***, G. Llewellyn, J. Westland, D. Yotheimer, P. Grievé, T. Sowers, E. Humston-Fulmer, S. Brantley

9:00 – 1207. Congener-specific determination of mono- to trichlorinated naphthalenes by comprehensive 2D gas chromatography/mass spectrometry. **N. Hanari***, J. Falandyz, G. Petrick, N. Yamashita

9:20 – 1208. Profiling and quantifying short chain chlorinated paraffins using comprehensive 2D gas chromatography with high resolution time-of-flight mass spectrometry. **L. Gao**, D. xia, M. Zheng

9:40 – 1209. Tracing of VOC composition of flower, honey, mead, and distillate made from linden by GCxGC-TOF MS. **I. Špánik***, L. Bulavová, O. Vyvierska, P. Szolcsányi

10:00 – 1210. Comprehensive 2D hydrophilic interaction chromatography × reversed phase liquid chromatographic analysis of phenolics: Theory, practice, and applications. **A. de Villiers***, K.M. Kalili, C.M. Willems, A.G. Tredoux, M.A. Stander, J. Vestner

10:20 – 1211. Development of comprehensive LCxLC and LCxCCE platforms containing In-line enzymatic degradation reagents for advanced oligonucleotide characterization. **F. Lyne**

10:40 – 1212. Use of quantitative structure-retention relationships to choose the optimal chromatographic techniques in 2D liquid chromatography. **P.R. Haddad***, S. Park, R.A. Shellie, M. Taraji, Y. Wen, M. Talebi, R. Amos, R. Szucs, C. Pohl, J. Dolan

11:00 – 1213. Compatibility study and impurity identification of a parental drug microdose formulation by 2DLC-MS. **L. Dai***, K. Zhang

11:20 – 1214. Development of a rapid LC-MS/MS screening method for illegal and counterfeit drugs: From 24 synthetic and natural cannabinoids to 82 erectile dysfunction treatments and adulterated products. **K.C. Waldron***, P. Lebel, A. Furtos

Marriott Waikiki Beach
Milo IV / V

Novel Analytical Probes for In Vivo Optical Functional Imaging (#115)

Organized by: Y. Urano, T. Ozawa, Y. Chang, M. McCarroll

Presiding: M. McCarroll

8:00 – 1215. Electrophysiology: Unplugged - small molecule fluorescent voltage sensors for studying membrane potential. **E. Miller***

8:25 – 1216. Development of response selective and tunable fluorescent probes. **M. McCarroll***, C.N. Scott, Q. Best

8:50 – 1217. Near-infrared and long-wavelength fluorescent probes. **R. Strongin***, L. Wang, S. Gibbs, H. Li, M. Siberian-Vazquez, M. Lowry, J. Escobedo

9:15 – 1218. Glutathione-targeted reversible fluorescent probes for real-time monitoring in living cells. **K. Umezawa**, M. Yoshida, M. Kamiya, Y. Urano*

9:35 – 1219. Design and synthesis of RNA-binding fluorescent ligands for siRNA delivery imaging. **S. Nishizawa***

10:00 – 1220. Design of an ultra-sensitive fluorescent probe composed of artificial nucleic acid for visualization of RNA in living cell. **K. Murayama**, Y. Kamiya, H. Kashida*, H. Asanuma*

10:20 Break

10:35 – 1221. Spatiotemporal mapping of temperature in living systems with molecular fluorescent thermometers. **S. Arai***, M. Suzuki, Y. Chang

10:55 – 1222. Diced electrophoresis gel assay for screening enzymes with specified activities. **T. Komatsu**, J. Onagi, A. Nakada, Y. Urano

11:15 – 1223. Artificial reaction promoter and bioparticle chemistry. **H. Komatsu***, Y. Shindo, K. Oka, M. Kanai, J. Hill, K. Ariga

11:35 – 1224. Fluorescent pH probes with tunable photophysical properties: Applications in cellular imaging. **C.N. Scott***, Q. Best, c. Liu, M. McCarroll

Marriott Waikiki Beach
Kona Moku BlrM A

Marine and Freshwater Toxins: Detection, Structure, and Pharmacology (#138)

Organized by: T. Tsumuraya, J. Hungerford, R. Lewis

Presiding: R.J. Lewis

8:00 Introductory Remarks

8:05 – 1225. Analysis of saxitoxin and its analogs by hydrophilic interaction liquid chromatography-tandem mass spectrometry (HILIC-MS/MS). **M.A. Quilliam***, D. Beach, K. Thomas, P. McCarron

8:45 – 1226. Toxin and species identification of marine toxins-implicated into recent food poisonings in Taiwan. **D. Hwang**

9:25 – 1227. Screening and structure elucidation of the possible biosynthetic intermediates of tetrodotoxin from the newts. **Y. Kudo**, Y. Cho, K. Konoki, M. Yotsu-Yamashita*

9:45 – 1228. Effects of brevetoxins on the neurotransmitters profile of the central nervous system of marine Medaka (*Oryzias melastigma*). E.N. LEI, M. YAU, C. YEUNG, **H. Lam***

10:05 Break

10:15 – 1229. Structural characterization of new peptide variants produced by cyanobacteria from the Brazilian Atlantic Coastal Forest using liquid chromatography coupled to quadrupole time of flight tandem mass spectrometry. **E. Pinto**, **M. Roldan**

10:35 – 1230. Our recent studies of tetrodotoxin, saxitoxin and polycavernosides. **M. Yotsu-Yamashita***, Y. Kudo, S. Tsuchiya, K. Maeta, Y. Cho, K. Konoki

11:15 – 1231. In vivo and in vitro effects of new palytoxin analogs. **A. Tubaro**, M. Pelin

11:55 Closing Remarks

Marriott Waikiki Beach
Waikiki BlrM III

Paper-Based Analytical Devices for Point of Need Measurements (#213)

Organized by: D. Citterio, C. Henry, J. Brennan

Presiding: J.D. Brennan, D. Citterio

8:00 – 1232. Enzyme-based signal amplification for paper-based assays for influenza A detection. **K. Abe**, P. Yager*

8:15 – 1233. Paper-based ELISA for E.Coli detection. **M. Hsu**, C. Cheng*

8:30 – 1234. Paper or plastic? Paper.

C.D. GARCIA, E. Evans, E. Costa, E. Moreira, W. Coltro, C. Do Lago

9:00 – 1235. Reagentless enzyme based paper sensors for field monitoring: From basic research to practical applications. **S. Andreescu***

9:20 – 1236. Extending the reach of molecular diagnostics: a paper-based sample-to-result platform. **B. Lutz**, P. Yager

9:50 Break

10:00 – 1237. Sample transport behaviour in paper-based biosensors. **W. Shen**

10:30 – 1238. Indirect antiglobulin paper test for red blood cell antigen typing. **N. Yeow***, H. McLiesh, W. Shen, G. Garner

10:50 – 1239. Microfluidic paper-based sensors for clinical and environmental diagnostics. **C. Henry**, J. Volckens, D. Cate, J. Adkins, J. Mettappoonipak, K. Boehle

11:10 – 1240. Development and optimization of paper-based analytical devices (μ PADs). **F.A. Gomez***, M. Arrastia, A. Avoundjian, F. Tsai, M. Jalali-Heravi, H. Valadez

11:30 – 1241. Paper, plastic, and a mobile app: Cost-effective, world-ready tools for distributed diagnostics. **V.T. Remcho**

Marriott Waikiki Beach
Kona Moku BlrM C

Analytical Laser-Induced Breakdown Spectroscopy (LIBS) for Hazards Analysis, Forensics, and Health (#379)

Organized by: J. Almirall, Y. Deguchi, A. Mizolek, S. Rehse, Z. Wang

Presiding: J. Almirall

8:00 – 1242. Capabilities of tandem LIBS and LA-ICP-MS for elemental analysis of samples of environmental, health and forensic interest. J. Gonzalez, D. Quarles, D. Oropesa, **R.E. Russo**

8:40 – 1243. Recent LIBS-enhancement techniques applied toward isotopic-composition analysis. C. Akpovo*, J. Martinez, A. Ford, S. Brown, L. Johnson

9:10 – 1244. Cylindrical cavity confined laser induced breakdown spectroscopy for improvement of signal intensity and stability. **W. Zhou***

9:40 – 1245. Progress and challenges in using LIBS for bacteriological identification. **S.J. Rehse***, D. Malenfant, D. Gillies

10:10 Coffee Break

10:30 – 1246. Selected application of laser-induced breakdown spectroscopy (LIBS). K. Novotny, J. Novotny, D. Prochazka, P. Porizka, A. Hrdlicka, G. Vitkova, **J. Kaiser***

11:00 – 1247. Determination of lanthanide elements in LiCl-KCl eutectic salt using laser-induced breakdown spectroscopy. **T. Kim***, J. Chung, S. Park, J. Yun

11:30 – 1248. New developments in forensic applications of LIBS. **J. Almirall**

Marriott Waikiki Beach
Waikiki BlrM I

Advances in Analytical Techniques for Effective Food Allergen Management (#394)

Organized by: N. Lee, S. Godefroy, S. Taylor, H. Akiyama, J. Baumert, M. Shoji

Presiding: J. Baumert, M. Shoji

8:00 – 1249. Effects of processing and food matrix on almond (*Prunus dulcis*) detection using murine monoclonal antibody-based sandwich enzyme-linked immunosorbent assay. **S.K. Sathe***, G.S. Chabba, C. Liu, V. Zaffran

8:30 – 1250. Enzyme-linked immunosorbent assay to detect food allergens in processed foods in Japan. **R. Adachi***, S. SAKAI, H. Akiyama, T. NISHIMAKI-MOGAMI

9:00 – 1251. PCR methods for detecting food allergens by using DNA sequences for species classification. **T. Hirao***

9:30 – 1252. PCR methods for wheat, buckwheat and soybean. **H. Yamakawa**

9:55 Break

10:10 – 1253. Hazelnut (*Corylus avellana*) detection using a monoclonal antibody-based direct sandwich enzyme-linked immunosorbent assay. **S. Gupta**, C. Liu, V. Zaffran, Q. Zhao, S.K. Sathe*

10:30 – 1254. Impacts of thermal and non-thermal processing on the immunoreactivity of parvalbumin from Southern Hemisphere fish species. **J. Liang***, S. Muralidharan*, S.L. Taylor, J. Baumert, A. Lopata, N.A. Lee*

10:50 – 1255. Immunoreactivity of pistachio proteins assessed by a monoclonal antibody-based enzyme-linked immunosorbent assay. **C. Liu**, J. Zhao, S. Alasvand Zaravandi, S.K. Sathe*

11:10 – 1256. Pecan (*Carya illinoensis*) detection using a monoclonal antibody-based direct sandwich enzyme-linked immunosorbent assay. **V. Zaffran**, C. Liu, S. Gupta, Q. Zhao, S.K. Sathe*

11:30 Closing

* Principle Author

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Marriott Waikiki Beach
Milo III

Organized Surfactant Assemblies in Chemical Analysis and Separation Science: Fifty Years Later (#457)

Organized by: W. Hinze, T. Saitoh,
G. Jiang, J. Liu
Presiding: W. Hinze, Y. Takagai

8:00 – 1257. Bio- and chemiluminescence analyses in liposomal media. **H. Tani***, A. Ishida, M. Tokeshi

8:40 – 1258. Microfluidic droplet operations utilizing spontaneous emulsification. **A. Hibara***, M. Fukuyama

9:20 – 1259. Surfactant assemblies-based fluorescent sensors with discrimination ability. **L. Ding***, Y. Cao, S. Wang, Y. Fang

10:00 – 1260. Separation and recovery of Beryllium based on pH-sensitive polymer as functional separation media. **T. Kato**, S. Igarashi

10:40 Concluding Remarks

INOR

Area 2 – Inorganic

Tuesday Morning

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Organic-Main Group Avenues toward Advanced Materials (#16)

Organized by: T. Baumgartner, S. Liu, S. Yamaguchi
Presiding: T. Baumgartner

8:00 Opening remarks

8:10 – 1. Phosphorus-containing fluorophores for bioimaging. **S. Yamaguchi**

8:30 – 2. Molecular engineering of boron(III) complexes for organic photovoltaics applications. **R. Ziesel***

9:00 – 3. Phosphorous(V)-phthalocyanines emitting intense fluorescence in the optical therapeutic window. **H. Isago***, H. Fujita, T. Sugimori

9:20 – 4. Designed hybrid organic-inorganic nanobuilding blocks from nucleophilic substitution reactions and their applications. **V. Ervithayasuporn***

9:40 – 5. Main group based single source precursors for MOCVD processes and for the generation of nanocystals. **M. Scheer***, C. Grassl, S. Bauer, S.B. Clendenning, P.E. Romero

10:10 Break

10:20 – 6. Synthesis and optical properties of 3-coordinate organoboron compounds. **T. Marder***

10:50 – 7. Solid-state emissive organoboron-based biphenyl system with large Stokes shift. **C. Zhao***

11:10 – 8. Novel phosphaphenalene derivatives: A non-catalyzed protocol to access fused phosphorus heterocycles. **C. Romero-Nieto***, A. Lopez-Andarias, C. Egler-Lucas, P. Hindenberg

11:30 – 9. Advances in phosphate based molecular materials. **M. Hissler***

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Fundamentals and Applications of Solvent Extraction in the Recovery of Strategic Metals (#17)

Organized by: A. Chagnes, J. Lee, N. Welham, B. HAY
Presiding: A. Chagnes

8:00 Opening remarks

8:05 – 10. Strategies for diversifying the supply of critical materials through the development of new separation technologies for rare earths. **B.A. Moyer***

8:25 – 11. Liquid-liquid extraction of rare earth elements by ionic liquid. A. Kumari, M.K. Sinha, **S.K. Sahu***, B.D. Pandey
8:45 – 12. New extractants applicable to industrial solvent extraction for the recovery of strategic metals. **M. Goto***, Y. Baba, F. Kubota

9:05 Break

9:15 – 13. Extraction of selected lanthanides from aqueous hydrochloric acid media using N, N', N' - tetrabutylidiglycolamide (TBDGA) in octanol and TBDGA in supercritical fluid carbon dioxide. **M.E. Mincher***, R.V. Fox, B.J. Mincher, D.L. Baek, C.M. Wai

9:35 – 14. Important selected issues regarding lanthanides and noble metals liquid-liquid separation. **D. Meyer**, D. Bourgeois, R. Poirot

9:55 – 15. Solvent extraction and solid phase extraction of rare earth elements using functionalized adsorbents from saline solutions. **A. Karamalidis***, C.W. Noack, K. Perkins, N. Washburn, D.A. Dzombak

10:15 Break

10:25 – 16. Extraction by preorganized tridentate analogs of synergistic hydroxoxime/carboxylate mixtures. J.W. Roebuck, B. Turkington, D.M. Rogers, G.S. Nichol, V. Cocalia, A. Fischmann, M. Pelser, S. Parsons, **P. Tasker***

10:45 – 17. Probing redox-facilitated phase transfer mechanisms in solvent extraction using voltammetry. **R. Ellis***

11:05 – 18. Fundamental studies of metal ion partitioning in ionic liquid-based solvent extraction systems employing neutral extractants. **M.L. Dietz***

11:25 Closing remarks

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65)

Organized by: T. Autrey, D. Stephan, z. Wang
Presiding: T. Autrey, D. Stephan, Z. Wang

8:00 Introductory Remarks

8:05 – 19. New avenues in FLP chemistry. **D. Stephan**

8:35 – 20. Catalytic Si-H bond activation with Lewis acids. **M. Oestreich**

9:05 – 21. Al/P based frustrated Lewis pair as an effective ambiphilic ligand. **W. Uhl***, J. Backs, P. Wegener

9:35 – 22. Reactivity of a neutral tricoordinate organoboron as a nucleophile. **R. KINJO***

10:05 Break

10:10 – 23. Cationic carbon Lewis acids in frustrated Lewis pairs. **M.J. Ingleson**

10:35 – 24. Activation of alkynes with $B(C_6F_5)_3$: Intramolecular cyclization reactions and rearrangements. **R. Melen***

11:00 – 25. Cooperative Lewis acid/base catalysis. **J. Slootweg**

11:25 – 26. New avenues for frustrated Lewis pair hydrogen activation: Synthesis and reactivity of boron-based radicals. **L. Longobardi***, D. Stephan*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Molecular Catalysis of Water Splitting Reactions (#76)

Organized by: K. Sakai, L. Sun, G. Brudvig, L. Spiccia
Presiding: L. Sun

8:00 – 27. Photocatalytic water oxidation by molecular metal oxides mimicking the natural oxygen evolving center. **M. Bonchio***

8:30 – 28. Molecular oxidation catalysis with iridium: Water splitting and CH-oxygenation. **U. Hintermaier***, S. Sheehan, J. Thomsen, G. Brudvig, R. Crabtree

8:50 – 29. Pathway for oxygen-oxygen bond formation and O_2 release in water oxidation catalyzed by dinuclear Ru complex. **K. Tanaka***

9:20 – 30. Unraveling solution speciation and stability of cobalt-polyoxometalate water oxidation catalysts by X-ray scattering. **S. Goberna Ferron***, J. Soriano-Lopez, M. Nyman, J. Galan-Mascaros

9:40 Coffee Break

10:00 – 31. Ruthenium complexes with carboxylate ligands as highly efficient molecular catalysts for water oxidation. **L. Sun**

10:30 – 32. New series of dinuclear ruthenium(II) complexes toward an active water oxidation catalyst prompting intramolecular O-O bond formation. **M. Yagi***

11:00 – 33. Molecular catalyst for water oxidation and oxygen reduction. **A. Liobet***

11:30 – 34. Water oxidation catalyzed by multinuclear metal complexes. **S. Masaoka**

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Frontiers of Organo-f-element Chemistry (#125)

Organized by: F. Edelmann, P. Diaconescu, Y. Chen, D. Emslie, P. Junk
Presiding: F. Edelmann

8:00 Introduction

8:10 – 35. Structure determination of uranocene and the first COT lanthanide complexes. **K.N. Raymond**

8:40 – 36. Low valent f-element chemistry: A theoretical journey. **L. Maron**

9:10 – 37. Bond strength in organo-f-element compounds from the quantum theory of atoms-in-molecules. Q. Huang, N. Kaltooyannis*

9:30 – 38. Magnetic personality of lanthanide ions. **M. Murugesu**

9:50 Coffee break

10:00 – 39. Redox and photoredox chemistry of cerium coordination complexes. **E.J. Schelter***

10:20 – 40. Reduction chemistry of rare-earth metal complexes supported by ferrocen diamide ligands. **P.L. Diaconescu**

10:40 – 41. Pentadienyl-supported rare-earth metal tetramethylaluminate complexes. **D. Barisic**, C. Maichle-Mössmer, R. Anwander

11:00 – 42. Steric effects in Sm(II) reduction chemistry illustrated with pyrrolide-based macrocyclic ligands of variable conformational flexibility. **M.G. Gardiner***

11:20 – 43. Star-driven Ce(IV)/Ce(II) redox couple within the fullerene cage. **A. Popov***, Y. Zhang

11:40 – 44. Gadolinium endohedral metallfullerenes: Next generation magnetic resonance imaging contrast agents. **H.C. Dorn***

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Non-covalent Interactions in Coordination Systems (#161)

Organized by: T. Konno, K. Lu, A. Hor
Presiding: T. Konno

8:00 – 45. Non-covalent interactions in coordination systems. **T. Konno***

8:10 – 46. Non-covalent interactions in extended architectures derived from transition metal complexes of bis-diketone and bis-triketone ligands: From polyrotaxane generation to pressure induced molecular switching. **L.F. Lindy***

8:30 – 47. Ag- π interactions in heterometallic dipyrrom based coordination networks. **S. Baudron***, H. Ruffin, M. Hosseini

8:50 – 48. Thyminate(2-)bridged cyclic tetranuclear rhodium(III) complexes formed by a template of a sodium, calcium or lanthanoid ion. **T. Suzuki***, A. Kashima, M. Sakata, H. Ota, A. Fuyuhiro, Y. Sunatsuki

9:05 – 49. Synthesis and properties of amido- and imido-gold(III) complexes having polypyridyl ligands. **K. Tsuge***, S. Iwashita, Y. Saito, T. Yada, H. Ohtsu

9:20 – 50. Flexible crystals: Stretching the boundaries of a single crystal. **J.K. Clegg***, J. McMurtie, A. Worthy, M. Pfrunder, A. Grosjean, A. Brock

9:35 – 51. Syntheses and luminescent properties of neutral Z-shaped heteropoly-nuclear platinum(III) complexes. **K. Umakoshi***, M. Ueda, K. Nishihara, Y. Nakao, Y. Arikawa

9:50 Break

10:00 – 52. Exploring the fundamental nature of non-covalent interactions in chemistry. **P. Kennepohl***, C. Mustoe

10:15 – 53. Modulation of emission properties of pincer Pt complex by intermolecular interactions. **J. Kuwabara**, K. Yamawaki, T. Kanbara

10:30 – 54. Targeting biomolecules with photoactive ruthenium(II)-based metallocacycles. **J. Thomas**

10:45 – 55. Chromic behavior and coordination structure conversion of hydrazone-palladium(II) and platinum(II) complexes in the solid state and in solution. **K. Nakajima**

11:00 – 56. Supramolecular chemistry of gold clips. **J. Yip***

11:20 – 57. Unusual coordination modes of hydrides identified from Cu(I) clusters supported by dichalcogenolates. **C. Liu**

11:40 – 58. From discrete low-dimensional metal complexes to supramolecular assemblies. **V. Yam**

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186)

Organized by: M. Hirano, D. Fogg, A. Veige
Presiding: A.S. Veige

8:00 – 59. Cobalt catalyzed C-H functionalization. **P.J. Chirik***

8:20 – 60. Bond activation reactions by highly reduced late-metal organometallics. **J.S. Figueira**, C. Mokhtarzadeh, A.E. Carpenter

8:40 – 61. Ruthenium(II) catalysts for C-H bond activation and functionalization. **P.H. Dixneuf***, P.B. Arcockiam, B. Li, F. Pozgan, K.S. Singh, C. Bruneau

9:00 – 62. Computational studies of Ru(II)-catalysed direct aryl- and alkylation: Novel C-H and C-I bond breaking and C-C bond making processes. **S.A. Macgregor***, K.J. Carr, C.L. McMullin

9:20 – 63. Experimental and computational characterization of bimetallic reaction pathways relevant to catalysis. **N.P. Mankad**

9:40 – 64. Synthesis and N-H reductive elimination study of dinuclear ruthenium imido dihydride complexes. **S. Takemoto***, H. Matsuzaka*

10:00 break

10:10 – 65. Catalytic α -acylalkylation at ortho C-H bond in arenes with cyclic alkyl carbonates. **F. Kakiuchi**

* Principle Author

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- 10:30 – 66.** Rh(II)-Rh(II) vs Rh(II)-Rh(III) complexes as catalysts in metal nitrene/nitrenoid reactions. **H. Lebel***, H. Piras, J. Bartholoméus
- 10:50 – 67.** Rhodium(I)-catalyzed cyclopropanation/cyclization of allene-ynes via rhodacycle-directed sp³-C-H activation. **Y. Sato***
- 11:10 – 68.** Synthesis and characterization of an osmium(II) methane coordination complex. P.J. Sempsrott, C.F. Lovitt, **G.S. Girolami***
- 11:30 – 69.** Si–H bond activation via σ -interaction in a cobalt(II) complex. **J. Kim**, K. Park, S. Kim, Y. Lee*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

New Frontiers in Bioinorganic Chemistry (#356)

Organized by: M. Yamaguchi, S. Cohen, X. Ottenwaelder
Presiding: K. Franz, T. Storr

- 8:00** Opening remarks
- 8:05 – 70.** Geometric and electronic structural contributions to Fe/O₂ reactivity. **E.I. Solomon***
- 8:35 – 71.** Defining a preference for polarizable halogen substituents in the hydroquinone ring-cleaving dioxygenase PcpA. **T.E. Machonkin**
- 8:55 – 72.** Mechanistic and biophysical characterization of oxalate decarboxylase. W. Zhu, J. Wilcoxen, L. Easthon, T. Stich, R. Britt, K. Allen, **N. Richards**
- 9:15 – 73.** Toward a better understanding of liver alcohol dehydrogenase: Synthesis, characterization, and activity of zinc(II) model complexes based on bis-triazole and bis-imidazole precursors. **J.R. Miecznikowski***, M. Lynn, W. Lo, J.P. Jasinski, S. Jain
- 9:35 – 74.** Metal-catalyzed reactions of N,N'-disubstituted imidazolinium cations with hydrogen as functional models of hydrogenases in methanogenesis. **H. Seino***, M. Hatazawa, Y. Hojo, H. Suzuki, K. Takahashi, Y. Mizobe, N. Yoshie

9:50 Break

- 10:00 – 75.** Targeting cancer specific cellular processes with ruthenium compounds. **A. Nazarov***

- 10:20 – 76.** Overcoming platinum resistance using small-molecule antineoplastic agents. **I. Romero Canelón***, M. Mos, A. Knight, P.J. Sadler

- 10:40 – 77.** Bioinspired catalyst composed of cobalamin and semiconductor with vitamin B12 function. **H. Shimakoshi***, Y. Hisaeda

- 11:00 – 78.** Catalytic metallodrugs: Structure-function and activity studies of a broad therapeutic platform. Z. Yu, M.J. Ross, I. Fidai, **J.A. Cowan***

- 11:30 – 79.** Developing a research platform for the discovery of cytotoxic metal complexes. **E.P. Glazer***

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Dynamic Aspects of Solid Materials: From Equilibrium to Non-equilibrium Systems (#376)

Organized by: M. Kawano, B. Abrahams, M. Garcia-Garibay, L. Zheng
Presiding: B.F. Abrahams, M. Kawano

- 8:00** Opening remarks
- 8:05 – 80.** Negative thermal expansion in coordination framework materials. **C. Kepert***

- 8:35 – 81.** Dynamic structural transformations of coordination cage assemblages. **P. Larpent**, S. Furukawa*, S. Kitagawa*

- 8:55 – 82.** In-situ synchrotron X-ray diffraction study of successive crystallization in metal-organic frameworks. **H.H. Yeung***, Y. Wu, S. Henke, A.K. Cheetham, D. O'Hare, R.I. Walton

- 9:15 – 83.** Dynamic processes in electron-rich coordination networks. **B.F. Abrahams***, R. Elliott, R. Robson, A. Sutton

9:45 Break

- 9:55 – 84.** Kinetic assembly of porous coordination networks. **M. Kawano**
- 10:15 – 85.** Relief of forbidden catenation in a metal-organic framework: Network conversion from interpenetration-frustrated graft to interpenetration-allowed homopolymer. **M. Lah***
- 10:45 – 86.** Reaction dynamics in coordination polymers. **J.J. Vittal**
- 11:15 – 87.** Moving protons in metal organic frameworks. **G. Shimizu***, P. Ramaswamy, N. Wong, S. Kim, Z. Fard

Tuesday Afternoon

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Organo-Main Group Avenues toward Advanced Materials (#16)

Organized by: T. Baumgartner, S. Liu, S. Yamaguchi
Presiding: S. Liu

13:00 Lunch break

- 13:20 – 88.** Singlet carbenes for the stabilization of main group paramagnetic species. **G. Bertrand**

- 13:50 – 89.** Donor-acceptor stabilization of low-oxidation state main group hydrides: From chemical curiosities to viable precursors to functional nanomaterials. **E. Rivard***, A. Swarnakar, T.K. Purkait, J. Veinto

- 14:10 – 90.** Stabilization and "transition metal-like" reactivity of low oxidation state/low coordination p-block metal complexes. **C. Jones***

- 14:40 – 91.** Stabilization of reactive main group species by coordination to carbonyl-decorated carbenes. **T.W. Hudnall***, A. Ledet, K. Melancon, A. Torres

15:00 Break

- 15:10 – 92.** Low-coordination numbers, unusual bonding, and dispersion force effects. **P.P. Power**

- 15:40 – 93.** Single, double, triple, chains: New forays into boron–boron bond formation. **H. Braunschweig**
- 16:10 – 94.** Dynamic covalent chemistry of organoboron and silicon compounds. **M. Wagner***

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Fundamentals and Applications of Solvent Extraction in the Recovery of Strategic Metals (#17)

Organized by: A. Chagnes, J. Lee, N. Welham, B. HAY
Presiding: N.J. Welham

13:00 Opening remarks

- 13:05 – 95.** Extraction and separation technologies. **D. Dreisinger***

- 13:25 – 96.** Interfacial phenomena in solvent extraction. **G. Stevens***

- 13:45 – 97.** Solvent extraction of magnesium by Cyanex 272: Experimental study and modeling. **V. Weigel**, M. Dehestru^t, M. STAMBOULI, M. Gohin, D. Pareau, Y. Le Quesne

14:05 – 98. Solvent extraction from ammoniacal solutions - some new perspectives. **N.J. Welham***, G. Johnston, M.L. Sutcliffe

- 14:35 – 99.** Development of hydrometallurgical recovery process of antimony by controlling the metal complexes condition in Sb-Cl-OH aqueous solution system. **S. Ueno**, S. Yokoyama, K. Shinoda, H. Takahashi*, K. Tohji

- 14:55 – 100.** Separation of Zr(IV) and Hf(IV) by solvent extraction. **M. Lee**

15:15 Break

- 15:25 – 101.** Liquid-liquid extraction of Bi(III) and Sb(III) by neutral extractants from HCl/H₂SO₄ mixed media.

- M. Avila-Rodriguez***, L.A. Santiago-Santiago, J.A. Reyes-Aguilar, M.d. González, D.E. García-Rodríguez, L. Hernández-Perales, D.F. Cholico-Gonzalez

- 15:45 – 102.** Ditopic thioetheramide reagents for the selective recovery of platinum and palladium. **J. Love***, P. Tasker, C.A. Morrison, K. MacRuary, m. Wilson, R.J. Gordon, R. Grant

- 16:05 – 103.** Liquid-liquid extraction separation of scandium from zirconium with O,O-bis(2-ethylhexyl) hydrogen thiophosphate. **y. Nakai**, Y. Nakajima, S. Oshima, Y. Watanabe, Y. Komatsu, K. Fujinaga

- 16:25 – 104.** Extraction studies of platinum and iron from hydrochloric acid solution with N-2-ethylhexyl-bis(N-di-2-ethylhexyl-ethylamide)amine. **M. Maeda***, H. Narita, C. Tokoro, M. Tanaka, R. Motokawa, H. Shiwaku, T. Yaita

16:45 Closing remarks

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65)

Organized by: T. Autrey, D. Stephan, z. Wang
Presiding: Z. Wang

- 13:00 – 105.** Accurate quantum chemistry for frustrated Lewis pair systems. **S. Grimme**

- 13:30 – 106.** Frustrated N-heterocyclic carbene-silylum ion Lewis pairs. **M. Tamm***, E. Theuergarten, M.F. Silva Valverde

- 14:00 – 107.** Synthesis of bulky organoboranes and their application in frustrated Lewis pair chemistry. **H. Wang***

- 14:25 – 108.** New strategies for borane-catalyzed metal-free hydrogenation. **H. Du**

14:50 Break

- 14:55 – 109.** Intramolecular FLPs with different Lewis acid sites - reversible H₂ addition and more. **T. Repò***, K. Chernichenko, I. Pápai, B. Kótaí, V. Zhivonitko

- 15:20 – 110.** Catalytic reduction of polar substrates using Frustrated Lewis pairs: An operando calorimetry approach to measure kinetics and thermodynamics under catalytic operating conditions. **T. Autrey***

- 15:45 – 111.** Unsupported metal-only-Lewis pairs of zero-valent iron- and ruthenium carbonyl complexes. **C. Schneider**, H. Braunschweig*

- 16:10 – 112.** Applications of N-Heterocyclic carbene-silylum ion Lewis pairs in FLP chemistry and bond activations. **M.F. Silva Valverde**, E. Theuergarten, T. Bannenberg, M. Freytag, P. Jones, M. Tamm*

- 16:35 – 113.** α -CH acidity of alkyl-B(C₆F₅)₂ compounds – the role of stabilized borata-alkene formation in FLP chemistry. **C. Mück-Lichtenfeld**, P. Moquist, G. Chen, K. Bussmann, C.G. Daniliuc, K. Gerald, G. Erker*

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Non-covalent Interactions in Coordination Systems (#161)

Organized by: T. Konno, K. Lu, A. Hor
Presiding: T. Konno

- 13:00 – 131.** Coordination chemistry of poly-carbene ligands. **E. Hahn***

- 13:40 – 116.** Theoretical design of hydrogen-evolving molecular electrocatalysts.

- S. Hammes-Schiffer**
14:10 – 117. From molecular non-noble metal catalysts to catalytic nanomaterials for energy-efficient and cost-effective electrochemical H₂ production.

- M. Wang***, P. Zhang, L. Chen, Y. Yang, J. Shen, L. Sun

- 14:40** Coffee Break
- 15:00 – 118.** Molecular catalysts for Ni_xCo_yRh_zPt-based H₂ evolution and Ru_xCo_y-based O₂ evolution. **K. Sakai***
- 15:30 – 119.** Hydrogen evolution: bioinspired catalytic materials and artificial hydrogenases. **V. Artero***
- 16:00 – 120.** Photo- and electrochemical water oxidation: New water oxidation chemistry of ruthenium complexes with polypyridyl tetradeятadien ligands. **J.T. Muckerman***, D.E. Polansky, J.J. Concepcion, R.P. Thummel, E. Fujita
- 16:30 – 121.** Hybrid metal-organic phosphonate realizing improved electrochemical water oxidation. T. Zhou, **R. Xu***

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Frontiers of Organo-f-element Chemistry (#125)

Organized by: F. Edelmann, P. Diaconescu, Y. Chen, D. Emslie, P. Junk
Presiding: D. Emslie

- 13:00 – 122.** Molecular non-metallocene hydrides of rare earth metals. **J. Okuda**

- 13:30 – 123.** Main group molecules in 4f-metal chemistry. **P.W. Roesky***

- 14:00 – 124.** Lanthanoid transition metal bonding. **R. Kempe***

- 14:30 – 125.** Chemistry of the lanthanoids involving the very bulky tetraphenyl- and pentaphenyl cyclopentadienyl ligands. **P.C. Junk***

- 14:50 – 126.** Structural variations in Ln(T_nP_nR)₂ compounds and their consequence on stability and reactivity. **F. Edelmann, A. Sella, J. Takats**

15:10 Coffee break

- 15:20 – 127.** Rare-earth metalla-cyclopentadienes: Synthesis, structure, and reactivity. **W. Zhang**

- 15:40 – 128.** Rare-earth metal phosphinidene complexes: synthesis, structure, and reactivity. **P. Cui, Y. Lv, J. Zhou, X. Zhu, S. Wang***

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Organic Interactions in Coordination Systems (#161)

Organized by: T. Konno, K. Lu, A. Hor
Presiding: T. Konno

- 13:00 – 131.** Coordination chemistry of poly-carbene ligands. **E. Hahn***

* Principle Author

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13:20 – 132. Influence of host-guest interactions on self-assembly of metallo-supra-molecular systems. **M. Hardie***, J.J. Henkelis, F. Thorp-Greenwood, T. Ronson, C. Carruthers, C. Sumby
13:40 – 133. Tailor-made synthesis of multi-layered trimetallic cyclophanes via transannular π - π interactions. **O. Jung**, H. Lee

14:00 – 134. Immobilization of metal mercury using reusable sulfurbridged molybdenum complex. **H. Akashi***, S. Shimokawato, H. Aikoh, T. Shibahara

14:15 – 135. Universal mode of ion-pairing interaction of tetraalkylammonium ions: Application to inorganic species. **A.J. Fry***

14:30 – 136. Development of hydrogen-evolution catalysts by using first-row transition metal complexes with sulfur donor atoms. **M. Hirotsu***, K. Santo, T. Nakae, T. Matsunaga, J. Sanou, I. Kinoshita
14:45 – 137. Synergistic effect of B...N co-ordinate bonding and ring strain makes 2-APB an ideal drug with dual effect. **H. Dong***, W. Li, J. Sun, S. Li, M.L. Klein

15:00 Break

15:10 – 138. Photooxidation of cyclometalated palladium complexes to the corresponding sulfonato species. **T. Kawamoto**

15:25 – 139. Osmium(V)-oxo complexes: Bioinspired catalysts for alkene functionalization. **H. Sugimoto***

15:40 – 140. Architectural complexity within secondary coordination spheres. **A.S. Borovik**

16:00 – 141. Non-covalent interaction between germyl and bridging gemylene ligands in dinuclear palladium(I) complexes. **K. Osakada***

16:20 – 142. Host-guest chemistry in coordination cages: Functions from drug binding to catalysis. **M. Ward**, C. Hunter

16:40 – 143. Importance of the second coordination sphere and of conformational flexibility in hydrolase modeling. **P. Comba***

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186)

Organized by: M. Hirano, D. Fogg, A. Veige

Presiding: M. Hirano

13:00 – 144. Transition metal vinylidene mediated catalysis for use in organic synthesis. **C. Lee**

13:20 – 145. Recyclable hybrid Rh and Ir catalysts for C-X bond formation reactions. **B.A. Messerle***, C. Wong, A. Tregubov, D.B. Walker, A. Soeriadi, A. Kochanar, J.J. Gooding

13:40 – 146. Rh-catalyzed enantioselective synthesis of chiral 3-aryl-3-(pyrazol-1-yl)propanoic esters. **H. Wu***

14:00 – 147. N-Heterocyclic carbene ligands as supports for low valent cobalt: Synthesis and reactivity of $\text{Cp}^*\text{Co}(\text{P}_{\text{i}})$. **J. Andjaba**, K. Dalphon, **C. Bradley***

14:20 – 148. Transition-metal-catalyzed asymmetric allylic dearomatization reactions. **S. You***

14:40 Break
14:50 – 149. Asymmetry and anisotropy: Activation of H_2 by novel Rh *NNN*-pincer systems leading to remarkably upfield ^1H NMR chemical shifts. **M.T. Zamora**, M.M. Hanninen, C.S. MacNeil, J.P. Knott, P.G. Hayes*

15:10 – 150. Synthesis and investigating the chemical reactivity of stable indenyl-ruthenium complexes containing small organic ring. **H. Sung***

15:30 – 151. Long-tethered P-P ligand: Synthesis, complexation, and catalysis. **E. Kwan Huang**, Y. Kawai, S. Kamakura, M. Yamashita*

15:50 – 152. Ligand-assisted bond activation on nickel and iridium NCN-pincer complexes featuring non-innocent N-heterocyclic carbenes. R.M. Brown, Y. Jiang, D.A. Levenson, I.I. Fay, C.J. Roberts, J. Valius, H.M. Tuononen, J. Borau-Garcia, D. Spasuk, **R. Roessler***

16:10 – 153. Nickel complexes as catalysts for C—H bond stannylation: A novel mechanistic pathway for the formation of carbon–heteroatom bonds. **S.A. Johnson***, M. Elsby

16:30 – 154. Hydrocarbon-soluble, base metal “nanocatalysts” with precious metal-like reactivity. **J.M. Stryker***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

New Frontiers in Bioinorganic Chemistry (#356)

Organized by: M. Yamaguchi, S. Cohen, X. Ottenwaelder

Presiding: P.S. Donnelly, C.G. Hartinger

13:00 – 155. Synthesis of metal complexes designed to assist in diagnosis and therapy. **P.S. Donnelly***

13:30 – 156. Lanthanide complexes for the treatment of bone resorption disorders. **D. Weekes***, J. Cawthray, O. Sivak, M. lafrate, K. Wasan, C. Orvig

13:45 – 157. Water-synthesized Zn:Sr:Mn quantum dots for multiple biological detection and enzyme immobilization. J. Beltran-Huarcas*, **D. Diaz-Diestra**, D. Bracho-Rincón, J. Gonzalez-Feliciano, C.I. Gonzalez, B.R. Weiner, G. Morell

14:05 – 158. Dual mode binding of ruthenium/osmium arene anticancer complexes to DNA: Coordination and intercalation. **H. Liu***

14:25 – 159. Targeting small-molecules to treat Alzheimer's disease. **T. Storr***, M. Jones, L. Gomes, R. Vieira

14:55 Break

15:05 – 160. M_2L_4 coordination cages as potential drug delivery systems for anticancer agents. **A. Schmidt**, M. Hollering, A. Pöthig, A. Casini*, F. Kuhn*

15:20 – 161. From targeted organometallic anticancer agents to intracellular target identification. **G.C. Hartinger***

15:50 – 162. Mechanistic insight into hydrogen-atom transfer reactions by chromium(IV)-oxo complexes: What is controlling the reactivity? **H. Kotani***, S. Kaida, T. Ishizuka, T. Kojima

16:10 – 163. Multitasking organometallic complexes as therapeutics. **A. Castonguay***

16:30 – 164. Conditional surrender: Designing molecules to put biological metals in their place. **K. Franz***

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Dynamic Aspects of Solid Materials: From Equilibrium to Non-equilibrium Systems (#376)

Organized by: M. Kawano, B. Abrahams, M. Garcia-Garibay, L. Zheng

Presiding: M.A. Garcia-Garibay, L. Zheng

13:00 – 165. Correlated dynamics in 1D chains of molecular rotors.

M.A. Garcia-Garibay, S. Perez-Estrada, B. Rodriguez-Molina

13:30 – 166. Crystalline molecular gyroscopes having a five-membered hetero aromatic ring rotor. **W. Setaka***

13:50 – 167. Polar molecules in charge-transfer crystals: Acquired dynamic and dielectric properties. **J. Harada***, M. Ohtani, Y. Takahashi, T. Inabe

14:10 – 168. Creation of new metal nanoparticles having non-equilibrium phases based on the “crystal structure control” and “inter-element-fusion” strategies. **K. Kusada**, H. Kitagawa

14:40 Break

14:50 – 169. Cobalt phosphonates with tunable magnetic and proton conduction properties. **L. Zheng**

15:20 – 170. Single-crystal-to-single-crystal molecular domino transformations triggered by mechanical stimulation and solid seeding. **H. Ito***

15:50 – 171. Exploring the solid-state and dynamic behaviour in second sphere coordination chemistry. **J. Martí-Rujs***

16:10 – 172. Self-reproduction of giant vesicle emerged under non-equilibrium condition. **T. Sugawara***, K. Takakura, K. Kurihara, T. Toyota, K. Suzuki

16:40 – 173. Dynamic aspects of molecular arrangement in a porous crystal with multiple binding pockets. **S. Tashiro**, R. Kubota, M. Shionoya*

Wednesday Morning

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Organo-Main Group Avenues toward Advanced Materials (#16)

Organized by: T. Baumgartner, S. Liu, S. Yamaguchi

Presiding: S. Yamaguchi

8:00 – 174. Organophosphorus avenues toward functional conjugated materials. **T. Baumgartner***

8:20 – 175. Facile synthesis of 2-phosphaquinolines and 2-phosphaquinolin-2-ones. **M.M. Haley***, C.L. Vonnegut, A. Shonkwiler, M.M. Khalifa, L.N. Zakharov, D.W. Johnson

8:40 – 176. Phospha-acenes. **J. Protasiewicz**

9:00 – 177. New ligand platforms for coordination chemistry based on BN/CC isostericism. **S. Liu***, A. Baggett, S. Xu, C. McConnell

9:20 – 178. BN-functionalized conjugated oligomers, polymers, and macrocycles. **F. Jaekle***

9:50 Break

10:00 – 179. Boron containing heterocycles: Methods, properties, reactivity. **W.E. Piers**, J. Araneda, A. Houghton, M. Morgan

10:30 – 180. Trilithiosilane: Synthesis and property. **M. Ichinobe**, A. Mori, A. Sekiguchi

10:50 – 181. Ring expansion reactions with pentaphenylborole as a route to generate six and seven-membered boracycles. **K. Huang**, **C.D. Martin**

11:10 – 182. Novel silicon analogs of stafanes that shows significant interactions between bridgehead silicon–silicon bonds. **T. Iwamoto**, A. Karube, S. Ishida

11:30 – 183. Phosphorus-analogues of pyromellitic diimides: A novel scaffold for creating organic electron-acceptors. **Y. Takeda***, K. Hatanaka, S. Minakata*

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Fundamentals and Applications of Solvent Extraction in the Recovery of Strategic Metals (#17)

Organized by: A. Chagnes, J. Lee, N. Welham, B. HAY

Presiding: G. Brudvig

8:00 Opening remarks

8:05 – 184. Recovery and extraction of strategic metals from WEEE – encountered challenges for hydrometallurgical route. **T. Retegan***, M. Gergoric, C. Tunsu, J. yang

8:25 – 185. Development of block copolymer extractants for the selective isolation of strategic metals. **L.A. Mitchell**, T.T. Nguyen, R.F. Fimognari, **B.J. Holliday***

8:45 – 186. Recovery of rare earth elements from fluorescent lamp waste fractions: Toward pilot scale separation. **C. Tunsu***, C. Ekberg, T. Retegan

9:05 Break

9:15 – 187. Solvent extraction recovery of nickel from electroless nickel plating baths. **M. Tanaka***, H. Narita, Y. Saiki, H. Naganawa

9:35 – 188. Efficient recovery of Ln from commercial lighting phosphors using acid adducts in scCO₂. **R.V. Fox***, D.L. Baek, M.E. Mincher, B.J. Mincher, C.M. Wai, C. Yen

9:55 – 189. Recovery of valuable metals from spent car NiMH batteries by leaching and solvent extraction. **M. Petranikova**

10:15 Break

10:25 – 190. Solvent extraction in the recovery of strategic metals from spent turbine-blade superalloy. **R.R. SRIVASTAVA**, M. Kim, **J. Lee***

10:45 – 191. Investigation of closed loop recycling of active materials for NiMH batteries. **F. Holmberg***, B. Ebin, M. Petranikova, B. Steenari, C. Ekberg

11:05 – 192. Intensification of interfacial transfer by forced vibration: Application to solvent extraction. **M. STAMBOULI***, D. Pareau, p. perre, N. Kozlov, V. Kozlov

11:25 Closing remarks

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65)

Organized by: T. Autrey, D. Stephan, z. Wang

Presiding: D. Stephan

8:00 – 193. Frustrated Lewis pairs as efficient catalyst for $\text{C}_{\text{sp}^2}\text{-H}$ bond activation. **F. Fontaine**, M. Legarde, M. Courtemanche, E. Rochette

8:30 – 194. Cis-stereoselective hydrogenation of acetylenes catalyzed by 2-amino-phenylboranes. **K. Chernichenko***, T. Repo, Á. Madarász, I. Pápai, M. Nieger, M. Leskelä

8:55 – 195. Kinetics of hydrogen activation on ceria-zirconia. **C. Sievers**, S.M. Schimmin, G. Foo , O.D. LaMont, A.K. Rogers, M.M. Yung, A.D. D'Amico

9:20 Break

9:25 – 196. On the origin of enantioselectivity of FLP-catalyzed asymmetric hydrogénations. **I. Pápai***, B. Kötai, A. Hamza, M. Lindqvist, T. Repo

9:50 – 197. FLP approach toward catalytic hydrogenation of CO₂. **E. Rochette***, M. Courtemanche, A. Pulis, M. Legarde, F. Fontaine, D. Stephan

10:15 – 198. Alane-based Lewis pairs in molecular catalysis and macromolecular synthesis. **E. Chen**

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Molecular Catalysis of Water Splitting Reactions (#76)

Organized by: K. Sakai, L. Sun, G. Brudvig, L. Spiccia

Presiding: G. Brudvig

8:00 – 199. Mechanisms of water oxidation in solution and on oxide surfaces. **T. Meyer***, M. Coggins, M. Sheridan, B. Sherman, N. Song, R. Binstead

8:30 – 200. Molecular catalysis in hydrogen evolution from water driven with low driving forces. **K. Yamauchi***, K. Kawano, K. Koshiba, K. Sakai*

* Principle Author

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<http://pacificifchem.org/>

onlineprogram

- 8:50 – 201.** Water oxidation pathways of bioinspired molecular cobalt catalysts. **G.R. Patzke***
- 9:20 – 202.** Developing functional hydrogenase mimics using model metalloprotein scaffolds. **H.S. Shafaat**, J. Slater, A. Manesis, H. Monaco
- 9:40** Coffee Break
- 10:00 – 203.** Water oxidation for solar fuel production. **G. Brudvig***, S. Sheehan, J. Thomsen, U. Hinternair, V. Batista, R. Crabtree, C. Schmutzlermaier
- 10:30 – 204.** Molecular and immobilized iridium catalysts for water oxidation. A. Bucci, I. Corbucci, L. Fagioli, G. Pastor, Z. Cristiano, **A. Macchioni***
- 11:00 – 205.** Homogeneous and heterogeneous pathways in water oxidation catalyzed by metal complexes. **T. LAU***
- 11:30 – 206.** Chemistry and materials biology approaches to artificial photosynthesis. **C.J. Chang***
- Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3
- Frontiers of Organo-f-element Chemistry (#125)**
- Organized by: F. Edelmann, P. Diaconescu, Y. Chen, D. Emslie, P. Junk
Presiding: P.C. Junk
- 8:00** Introduction
- 8:05 – 207.** (co)Polymerization of polar styrenes and styrene by rare-earth metal precursors. **D. Cui***
- 8:35 – 208.** Amido and alkyl rare-earth complexes for catalysis of intermolecular olefin hydrophosphination and hydroamination. **A. Trifonov***
- 9:05 – 209.** Rational development of metallorganic precursors of lanthanides and their application for thin film deposition of lanthanide oxides and lanthanide nitrides. **A. Devi***
- 9:25 – 210.** C-H bond activation and functionalization of *N*-heteroaromatics catalyzed by group 3 metal complexes. **K. Mashima***, H. Nagae, Y. Shibata, H. Tsurugi
- 9:55** Coffee break
- 10:10 – 211.** Rare-earth-catalyzed chain-end functionalization of syndiotactic polystyrene. **Z. Hou***
- 10:40 – 212.** Homogeneous imidazolin-2-imino acitindole catalysts. **M. Tam***, I.S. Karmel, M.S. Eisen, T. Bannenberg
- 11:00 – 213.** Synthesis and reactivity of rigid pincer ligand uranium alkyl complexes. **D. Emslie***, N. Andreychuk
- 11:20 – 214.** Cp₂U(NA)₂ complexes: Unusual electronic structure and unique reactivity. **J.M. Boncella***, N.C. Tomson, A.M. Tondreau, M. Winston, B.L. Scott
- 11:40 – 215.** Uranium oxide materials for solar hydrogen production. **S. Mathur**, J. Leduc
- Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2
- Non-covalent Interactions in Coordination Systems (#161)**
- Organized by: T. Konno, K. Lu, A. Hor
Presiding: A.T. Hor
- 8:00** Break
- 8:20 – 216.** Molecular recognition of Re-based metallocycles. **K. Lu***
- 8:40 – 217.** Supramolecular networking of macrocycles via exocyclic coordination. **S. Lee***
- 9:00 – 218.** Self-alignment of low-valent palladium chains. **T. Tanase***
- 9:20 – 219.** Effect of non-covalent weak interaction for helicity induction and dynamic inversion of chiral Co(II) complexes. **H. Miyake***
- 9:35 – 220.** Molecular balance for measuring weak metal-pi interactions. **K.D. Shimizu***
- 9:50** Break
- 10:00 – 221.** Synthesis, structures, and guest binding ability of multimetallic giant capsules. **M. Abe***, Y. Hisaeda

- 10:15 – 222.** Coordination chemistry of the indium(I) cation. **R.J. Wehmhschulte***, K. Osman, D. Powell
- 10:30 – 223.** Structural and chemical transformation of dihydrogen bond in an iron-based molecular electrocatalyst. **X. Wang***, R. Bullock, T. Liu
- 10:45 – 224.** Synthesis and coordination chemistry of molecular and polymeric Wurster-type, redox-active receptors. **J. Siber***
- 11:00 – 225.** Weak metal-ligand interactions involving hemilabile ligands. **W. Kaim***
- 11:20 – 226.** Phase transition and single-crystal-to-single-crystal transformation of d¹⁰-metal coordination architectures. **B. TZENG***
- Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2
- Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186)**
- Organized by: M. Hirano, D. Fogg, A. Veige
Presiding: M. Hirano
- 8:00 – 227.** Silver bullet: Catalytic nucleophilic additions, reductions, hydrogenations, and oxidations in water. **C. Li***
- 8:20 – 228.** Reductive elimination from high-valent transition metal complexes. **T. Ritter**
- 8:40 – 229.** Adding ligand-and-main group element dimensions to the C-H bond activation. **T. Ong**
- 9:00 – 230.** Pincer-crown ether complexes for cation-modulated bond activation and catalysis. **A. Miller***, M. Kita, J. Smith
- 9:20 – 231.** Development of hexa-*peri*-hexa-azobenzocoronene substituted "click" 1,2,3-triazole ligands for catalysis. **J.D. Crowley**, J.R. Wright, N.T. Lucas
- 9:40 – 232.** Novel carbon–hydrogen bond activation strategy based on interaction between an alkyne group and a palladium catalyst. **Y. Minami***, T. Hiayama*
- 10:00** Break
- 10:10 – 233.** Carbonylative esterification of primary alcohol with aryl chloride through Pd-promoted C-C bond cleavage. **C. Jun***, D. Kim, H. Park
- 10:30 – 234.** Nickel(0)-catalyzed transformation reactions viaaza-nickelacycle intermediates. **S. Ogoshi***
- 10:50 – 235.** Efficient C-H activation of arenes by a photoactivated Ni^I(azide). **J. van der Vlugt***
- 11:10 – 236.** Nickel-catalyzed C-F bond alkylation of acyl fluorides. **Y. Okuda**, J. Xu, Y. Nishihara*
- 11:30 – 237.** Proton shuttling pyridylphosphine ligands produce highly active catalysts for methoxycarbonylation. **T.A. Shuttleworth**, T.P. Turner, P.G. Pringle*
- Hilton Hawaiian Village
Kalia Tower, Hibiscus 2
- Nuclear Probes in Nanoscale Characterization (#254)**
- Organized by: M. Takahashi, A. Hill, V. Sharma, J. Wang, M. Takahashi, M. Takahashi, K. Nomura, Y. Yamada
Presiding: A.J. Hill, Y. Yamada
- 8:00 – 238.** Positron annihilation lifetime spectroscopy studies of nanomaterials. **A.J. Hill**, H. Thornton
- 8:40 – 239.** PALS: Unraveling polymer nano additive composites interactions over time. **K. Konstas***, C. Lau, M.R. Hill, A.J. Hill
- 9:00** coffee break
- 9:15 – 240.** Negative muon capture processes for low pressure gaseous molecules. **K. Ninomiya***
- 9:55 – 241.** Supertransferred hyperfine field at a unique residential site of ¹¹¹Cd in Fe₂O₃. **W. Sato***, S. Komatsuda, Y. Ohkubo
- 10:25** coffee break
- 10:40 – 242.** Optical switching and addressing of molecular switches in nanoscopic fibers. **F. Renz***, D. Unruh, M. Kumar, L. Heyer, T. Meyer, B. Dreyer, R. Sindlar, C. Krueger
- 11:20 – 243.** Ligand field strength of Fe(NC-S)(NCBH₃) unit for the assembled complexes bridged by 1,2-bis(4-pyridyl)ethane. H. Date, M. Kaneko, K. Inoue, S. Nakashima*
- 11:40 – 244.** Mossbauer spectroscopic study on Hofmann-like coordination polymer. **T. Kitazawa***, M. Sekiya, M. Takahashi
- Hilton Hawaiian Village
Rainbow Tower, Rainbow 1
- Metal-containing ?-Conjugated Systems: Syntheses, Properties, Applications (#269)**
- Organized by: M. Humphrey, V. Yam, M. Akita
Presiding: M. Akita, M. Humphrey
- 8:00** Opening remarks
- 8:05 – 245.** Organometallic single-molecule electronics: Tuning electronic transport and switching of mono- and dinuclear rigid-rod type acetylenic complexes. **H. Berke**
- 8:25 – 246.** Syntheses and nonlinear optical properties of metal alkynyl stars. **M. Humphrey***, T. Schwich, M. Cifuentes, M. Samoc
- 8:45 – 247.** Luminescent platinum(II) alkynyl system as π-capping metalloligand and chemosensors. **K. Wong***
- 9:05 – 248.** Metal acetylide complexes: New synthesis, wires, and sustainable chemistry. **T. Ren***, T. Cook, S. Natoli, S. Tyler
- 9:25 – 249.** Creating new activity of pi-conjugated systems by Pt insertion. **J. Yang***, C. Lin
- 9:45** Coffee break
- 10:00 – 250.** Charge delocalization vs. localization in carbon-rich iron mixed-valence complexes. **C. Lapinte**
- 10:20 – 251.** Single molecule conductance of molecular wires with redox-active organometallic units. **Y. Tanaka**, M. Akita
- 10:40 – 252.** Photochromic ruthenium alkynyl complexes as molecular switches. **M.C. Walkley**, L.T. Byrne, M.J. Piggott, P.J. Low, **G.A. Koutsantonis***
- 11:00 – 253.** Control of vinylidene rearrangement and 1,2-insertion of internal alkynes. **Y. Ishii***, Y. Ikeda, Y. Mutoh, S. Kodama
- 11:20 – 254.** Phosphorescent N-heterocyclic allynlidene metal complexes as building blocks for supramolecular polymeric nanomaterials and mesophases. **W. Lu***
- Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2
- Dioxygen Activation Chemistry of Metalloenzymes and Models (#339)**
- Organized by: A. Rosenzweig, S. Itoh, W. Nam
Presiding: A. Rosenzweig
- 8:00 – 255.** Biological methane oxidation. **A. Rosenzweig**
- 8:30 – 256.** Cu(II) in the oxidation of methane in pMMO? C.T. Citek, E. Wasinger, T.P. Stack
- 9:00 – 257.** Primary copper-dioxygen adducts: New platforms, substrate reactivity, and reduction. **K.D. Karlin***
- 9:30 – 258.** Copper-oxygen intermediates in oxidation catalysis. **W.B. Tolman***
- 10:00 – 259.** Geometric and electronic structure contributions to Cu/O₂ reactivity. **E.I. Solomon***
- 10:30 – 260.** Modeling reactive intermediates of copper monooxygenases. **S. Itoh**
- 11:00 – 261.** Construction of asymmetric mixed-valent dicopper(II,III) complexes as an active site model of multicopper oxidase. **H. Masuda**, T. Ochiai, T. Inomata, T. Ozawa
- 11:30 – 262.** Halide-promoted dioxygenolysis of a carbon-carbon bond in copper(II) diketonate complexes. **L.M. Berreau***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

New Frontiers in Bioinorganic Chemistry (#356)

Organized by: M. Yamaguchi, S. Cohen, X. Otterwaelder
Presiding: S. Ogura, M. Stillman

8:00 – 263. Metal-binding pharmacophores for metalloenzyme inhibitors. **S. Cohen**

8:30 – 264. Oximate metal complexes as models of hydrolytic metalloenzymes. **P. Gómez-Tagle***, J.C. Lugo-González, A.K. Yatsimirsky

8:50 – 265. New approach to the fluorescence imaging of platinum drug processing. **C. Shen***, L. Dawson, T. Hambley, E. New

9:05 – 266. Switching of photochemical ligand release on ruthenium complexes by external stimuli. **M. Yamaguchi***, T. Eguchi, A. Kobayashi, T. Masano, K. Sato

9:25 – 267. CO-eleasing molecules (CORMs) with targeted pharmacological activity. C. Mueller, C.G. Hartinger, L.J. Wright*

9:55 Break

10:05 – 268. Biogenic polyamines capture CO₂ and accelerate extracellular bacterial CaCO₃ formation. **K. Yasumoto***, M. Yasumoto-Hirose, J. Yasumoto, K. Mori-Yasumoto, M. Jimbo, T. Kusumi, S. Watabe

10:20 – 269. Model studies of acetyl CoA synthase catalyzing CO₂ fixation in organisms. **T. Matsumoto***, K. Tatsumi

10:40 – 270. Synthesis and properties of magnesium(II) complexes of sugar-conjugated fluorochlorin derivatives as new photosensitizers. **H. Akashi***, T. Sawada, K. Moriwaki, S. Yano

11:00 – 271. Metal induced folding in metallothioneins: New results and ideas from time-, temperature-, and modification-dependent ESI-MS studies. **M. Stillman***

11:30 – 272. Gene delivery system based on zinc-chelated imidazole groups for gene expression enhancement. **S. Asayama**

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

Isotope Production--Providing Important Materials for Research and Applications (#363)

Organized by: D. Phillips, K. Gagnon, Y. Hatsukawa
Presiding: K.D. John, D.R. Phillips

8:00 Opening Remarks--Dennis R. Phillips

8:05 – 273. Overview of the U.S. Department of Energy isotope program. **J.E. Gillo***

8:30 – 274. Preparation of radioisotopes for new medical use in Osaka University. **A. Shinohara***

8:55 – 275. Production of medical isotopes by photo-neutron reaction. **B. Szpunar**, C. Rangacharyulu, S. Daté, H. Ejiri

9:15 – 276. Production of ¹⁸⁶Re at the Brookhaven Linac Isotope Producer via proton induced reactions on natural tungsten and osmium targets. **M. Gott***, C. Cullen, L. Muñch, J. Nalepa, C.S. Cutler, A.R. Ketrin, D. Wilbur, S.S. Jurisson, S. Smith

9:35 Break

* Principle Author

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9:45 – 277. Nuclear workforce development – update on status of US training.
S.S. Jurisson*

10:10 – 278. Efficient method for recycling enriched ^{186}W target material used in the production of ^{186}Re via deuteron irradiation. **E. Balkin***, K.M. Gagnon, E. Dorman, R. Emery, B.E. Smith, K.T. Strong, P. Pauzauskie, M. Fassbender, C.S. Cutler, A.R. Ketring, S.S. Jurisson, D.S. Wilbur

10:30 – 279. High power accelerator targets for large scale production of radionuclides. **F.M. Nortier**

10:55 – 280. Recent developments in production and purification of novel PET isotopes. **S.E. Lapi***

11:20 – 281. Improved production of ^{89}Zr in a solution target. **M.K. Pandey**, J. Byrne, A. Packard, T. DeGrado

11:40 – 282. Production of $^{44}\text{Ti}/^{44}\text{Sc}$ generator at the Los Alamos Isotope Production Facility. **V. Radchenko***, J.W. Engle, D. Medvedev, J.R. Maassen, C.M. Narango, J.J. Wilson, E. Birnbaum, K.D. John, F.M. Nortier, M. Fassbender

Hawaii Convention Center
Halls I, II, III

Dynamic Aspects of Solid Materials: From Equilibrium to Non-equilibrium Systems (#376)

Organized by: M. Kawano, B. Abrahams, M. Garcia-Garibay, L. Zheng
Presiding: M. Kawano

Poster Session

10:00 – 12:00

283. Direct observation of growing process of MOF nanoparticles in solution by in-situ TEM. **T. Kikitsu***, H. Ohtsu, M. Kawano, D. Hashizume

284. Variation of morphology of K^+TPHAP^- single crystal surface in moisture by SEM observation. **D. Inoue***, G. Lee, Y. Yakiyama, M. Kawano, D. Hashizume

285. Dynamics and optical properties of a selenophene-bridged molecular gyrotrops in a crystalline state. **T. Masuda**, Y. Inagaki, K. Yamaguchi, W. Setaka*

286. Synthesis and birefringence of a molecular gyrotrop with a 4,4'-biphenylene rotator. **A. Fujiwara**, Y. Inagaki, K. Yamaguchi, W. Setaka*

287. Direct observation of enthalpy relaxation at around glass transition temperature. **J. Fujimura**, E. Nishiyama, I. Tsukushi*

288. Evaluation of thermodynamic fragility from heat capacity. **E. Nishiyama**, J. Fujimura, M. Yokota, I. Tsukushi*

Wednesday Afternoon

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Organo-Main Group Avenues toward Advanced Materials (#16)

Organized by: T. Baumgartner, S. Liu, S. Yamaguchi
Presiding: C. Romero-Nieto

13:00 Lunch Break

13:20 – 289. Creating conjugated materials via exciton-driven elimination reactions of BN-heterocycles. S.K. Mellerup, D. Yang, S. McDonald, S. Gong, Z. Lu, **S. Wang***

13:50 – 290. Fluorescent and photoisomerizable azobenzene by utilization of interactions between main group elements.

N. Kano*, M. Yamamura, T. Kawashima

14:10 – 291. Application of NHC pincer ligands in silicon chemistry. **M. Asay***

14:30 – 292. Synthesis, structure, and properties of organophosphorus polymers and materials derived from phosphphaalkenes. **D.P. Gates***

15:00 Break

15:10 – 293. Hypervalent pentacoordinated nitrogen radical cations: Synthesis, structure, and application to singlet diradicaloid. **Y. Yamamoto***, M. Takeshita, K. Sato, J. Nakatsuji, A. Kuroasaki, M. NAKANO, R. Kishi, K. Furukawa, K. Kamada

15:40 – 294. Lewis acidic organoantimony(V) derivatives: New approaches to anion sensing and organic reaction catalysis. **F. Gabai**

16:10 – 295. Isolation of anionic η^2 -sila-aldehyde-tungsten complexes. T. Fukuda, **H. Hashimoto***, H. Tobita

16:30 – 296. Synthesis, structures, and reactivity of stannole- and plumbole-based transition-metal complexes. **M. Saito***

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Fundamentals and Applications of Solvent Extraction in the Recovery of Strategic Metals (#17)

Organized by: A. Chagnes, J. Lee, N. Welham, B. HAY
Presiding: B.A. Moyer

13:00 Opening remarks

13:05 – 297. Physico-chemical study of uranium peroxide precipitation.

M. Bertrand*, E. Plasari, h. Muhr, F. Auger

13:25 – 298. Uranium(VI) chemistry in phosphoric acid media. A. Dartiguelongue*, **G. Cote***, A. Chagnes, E. Provost, W. Furst

13:45 – 299. ALSEP process kinetics testing and speciation studies. **A. Gelli***, M. Brown, G.J. Lumetta

14:05 – 300. Demonstration of innovative partitioning processes for minor actinide recycling from high active waste solutions. **G. Modolo***

14:25 Break

14:35 – 301. Overview of advanced minor actinides recycling processes developed in the United States. **P. paviet***

14:55 – 302. Advancing TALSPEAK chemistry. **K.L. Nash***

15:15 – 303. Chemistry of a combined extraction system for separation of trivalent actinides and lanthanides.

A. Paulenova*, B.J. Gullekson, A. Gelis

15:35 Closing remarks

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65)

Organized by: T. Autrey, D. Stephan, z. Wang
Presiding: K. Chernichenko

13:00 – 304. Overcoming inherent limits in frustrated Lewis pair catalysis: Moisture tolerant hydrogenations. **T. Soos***

13:30 – 305. Transition metal Lewis acid/base ensembles to promote cooperative substrate binding and activation.

N. Szymczak*, G. Ritch, E. Dahl, O. Tutusaus

14:00 – 306. Frustrated Lewis pair catalysed dehydrogenation and dehydrocoupling of Lewis acid/base adducts. **O. Metters**, D. Wass*, I. Manners*

14:25 – 307. FLP chemistry involving in the reversible dehydrogenation/hydrogenation of nitrogen heterocycle catalyzed by a $\text{C}_\text{p}\text{Ir}$ complex. **Z. Wang**

14:50 Break

14:55 – 308. Using free energies for H^+ and H^- transfers to design catalysts for the reduction of CO_2 . **A.M. Appel**, J. Linehan, E. Wiedner, B. Galan, M. Jeletic, C. Zall, S. Connally

15:20 – 309. Ferrocene-based planar chiral Lewis pair systems. **A. Tagne Kuate**, J. Chen, R.A. Lalancette, F. Jaekle*

15:45 – 310. Modification of borole compounds: An interplay between sterics and electronics. H. Braunschweig, H. Kelch*, L. Mailänder

16:10 – 311. Computational study of the donor-acceptor stabilization of low-oxidation state main group element hydrides.

A. Brown, E. Rivard, E. Antoniuk

16:35 – 312. Methanol dehydrogenation catalyzed by defined ruthenium pincer complex: Insights from a DFT study. **M. Lei***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Molecular Catalysis of Water Splitting Reactions (#76)

Organized by: K. Sakai, L. Sun, G. Brudvig, L. Spiccia
Presiding: L. Spiccia

13:00 – 313. Parallelization of water splitting photocatalysis. **R.S. Khnayzer***

13:20 – 314. Aminopyridine ligands as platforms for well-defined light-driven cobalt reduction and iron water oxidation catalysts. **D. Lloret Fillo***

13:40 – 315. Water oxidation catalysts derived from metal complexes. **L. Spiccia***

14:10 – 316. Noble-metal-free catalysts for hydrogen production and water oxidation: From molecular systems to nanomaterials. **P. Du**, Z. Sun, H. Chen, X. Liu

14:40 Coffee Break

15:00 – 317. Photocatalytic oxygen evolution by supramolecular assembly and semiconductor/molecular catalyst hybrid.

F. Li*, H. Li, Y. Wang, L. Sun

15:20 – 318. Photo- and electrochemical water oxidation with ruthenium polypyridyl complexes. **E. Fujita***,

J.J. Concepcion, J.T. Muckerman,

D.E. Polynsky, R. Thummel

15:50 – 319. Toward solar to fuel devices based on molecular components.

J.N. Reek

16:10 – 320. On how nickel electrodes mediate water oxidation. **C.P. Berlinguet***, R.D. Smith

16:40 – 321. Photoinduced electron transfer reaction at the solid-liquid interface: The importance of surface of nanoparticle-based photosensitizers. **A. Kobayashi***, K. Sawaguchi, E. Saitoh, M. Yoshida, M. Kato

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Frontiers of Organo-f-element Chemistry (#125)

Organized by: F. Edelmann, P. Diaconescu, Y. Chen, D. Emslie, P. Junk
Presiding: Y. Chen

13:00 – 322. Aspects of organocerium(IV) chemistry. **R. Anwander***, D. Schneider, J. Friedrich, C. Maichle-Mössmer, K.W. Törnroos

13:30 – 323. Recent advances in small molecule activation by organouranium complexes. **G. Cloke***

14:00 – 324. Bimetallic actinide complexes of constraining macrocycles for small molecule activation. **P.L. Arnold***, C. Stevens, R. White, M. Dutkiewicz, J. Barnaby, R. Caciuffo, C. Apostolidis, O. Walter, J. Love, M.G. Gardiner

14:30 – 325. Synthesis and reactivity of actinide-chalcogen multiple bonds.

D.E. Smiles, T. Hayton

15:00 Coffee break

15:10 – 326. Reactivity, molecular, and electronic structure of uranium coordination complexes in unusual geometries and oxidation states. **K. Meyer***

15:40 – 327. Ligand vs. metal centred redox reactivity of low valent f elements.

M. Mazzanti

16:10 – 328. Development of new ligand systems in actinide chemistry. **J. Arnold***

16:30 – 329. Recent advances in triamidoamine uranium-ligand multiple bonding.

S.T. Liddle, D. King, B. Gardner, P. Cleaves, A. Wooley, G. Balazs, M. Scheer, F. Tunai, E. McInnes, J. McMaster, W. Lewis, A. Blake

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Non-covalent Interactions in Coordination Systems (#161)

Organized by: T. Konno, K. Lu, A. Hor
Presiding: K. Lu

13:00 – 330. Isoreticular metal-organic frameworks based on a rhombic dodecahedral metal-organic polyhedron as a tertiary building unit. **M. Lah***

13:20 – 331. Cytocloricatechylene supramolecular assemblies. **B.F. Abrahams***, B. Boughton, J. Holmes, R. Robson

13:40 – 332. Spin state behaviour of iron(II)/dipyrazolylpyridine complexes: New insights from crystallographic and solution measurements. L.J. Kershaw Cook, T.D. Roberts, G. Sherborne, S. Alvarez, M.A. Halcrow*

14:00 – 333. Coordination polymers that convert to the discrete cage complexes for anions. **M. Kondo**, T. Inoue, S. Koike

14:15 – 334. Composite supramolecular frameworks: spin crossover in metal complexes encapsulated in halogen bonded networks. **J. McMurtie***, M. Pfrunder

14:30 – 335. Fluoride anion encapsulation into vanadium-oxygen cluster anion cages. **Y. Kikukawa**, Y. Hayashi*

14:45 – 336. Platinum to metal dative bond with third-row transition-metal d^{10} ion as an acceptor. **T. Yamaguchi***, H. Taniguchi

15:00 Break

15:10 – 337. Coordination chemistry of macrocycles assembled by supramolecular $\text{Te} \cdot \cdot \text{O}$ interactions. P. Ho, S. Jocelyn, L.M. Lee, I. Vargas-Baca*

15:25 – 338. Nonbonded interactions in bis(dinaphthylboryldimethylglyoximate)iron(II) complexes. **D.V. Stynes***, T. Doan

15:40 – 339. Synthesis of a helical trinickel(II) metallocryptand and regulation of its helix inversion rate by guest recognition.

S. Akine, M. Miyashita, T. Nabeshima

15:55 – 340. Supramolecular MOFs organized by flexible and robust $\pi \cdot \pi$ stacking interactions: Metal complexes with unusual structures and properties.

D. Reger*

16:10 – 341. Site-selective adsorption and dynamic behaviors of guest molecules in the nanochannel of metal-macrocycle framework. **M. Shionoya***

16:30 – 342. Creating new structural motifs by manipulation of hybrid ligand spacers.

A.T. Hor*

16:50 Concluding Remarks

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186)

Organized by: M. Hirano, D. Fogg, A. Veige
Presiding: D. Fogg

13:00 – 343. C-H borylation: The roles of experiment and theory in catalysis.

M. Smith

13:20 – 344. Unique bond cleavage and bond formation on the metal-boryl unit of PBP-type pincer iridium and rhodium complexes.

W. Shih*, W. Gu, M.C. MacInnis, O.V. Ozerov*

13:40 – 345. Choices of PC- and PCP-palladium catalysts for asymmetric P-H addition reactions.

P. Leung

14:00 – 346. Retrohydroformylation reaction.

S. Kusumoto, K. Nozaki*, T. Tatsuki

* Principle Author

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onlineprogram

14:20 – 347. Remarkable ligand effect of $P(2\text{-MeOC}_6\text{H}_4)_3$ on palladium-catalyzed direct arylation. **M. Wakioka**, Y. Nakamura, M. Michelle, F. Ozawa*

14:40 Break

14:50 – 348. Mechanistic insights into E-H activation reactions using palladium carbene complexes. **V.M. Iluc***

15:10 – 349. Chemoselective catalytic aerobic alcohol oxidation. **W.C. Ho***, A.J. Ingram, K. Chung, R. Waymouth

15:30 – 350. Reactions at high-oxidation state late transition metal centres generated from dicationic $\text{I}(\text{III})$ oxidants. **J.L. Dutton**

15:50 – 351. Model systems for unraveling fundamental redox processes of coinage metals in cross coupling catalysis. **X. Ribas***

16:10 – 352. Selective Negishi coupling of secondary alkylzinc reagents to aromatics: Solving the 5-membered ring heterocycle problem. M. Pompeo, B. Atwater, N. Chandrasoma, D. Mitchell, M. Rodriguez, F. Robert, **M.G. Organ***

16:30 – 353. Selectivity in Suzuki-Miyaura cross-coupling reactions. **C. Cradden***

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Nuclear Probes in Nanoscale Characterization (#254)

Organized by: M. Takahashi, A. Hill, V. Sharma, J. Wang, M. Takahashi, M. Takahashi, K. Nomura, Y. Yamada
Presiding: V. Sharma, J. Wang

13:00 – 354. Magnetic nanoparticles for targeted drug delivery. **V.K. Garg***, H.S. Loushambam, S.S. Pati, A.C. de Oliveira

13:40 – 355. Mössbauer studies of ferrite nanoparticles for reactive adsorption desulfurization. **C. Liang***

14:00 – 356. Appropriate ratio of metallic-iron and maghemite nanoparticles for environment purification. **Y. Watanabe**, S. Kubuki, K. Akiyama, M. Ristić, K. Stjepko, K. Erno, H. Zoltán, T. Nishida

14:20 Coffee break

14:30 – 357. Mechanism of iron nanoparticle formation in eukaryotic cells modeling Friedrich's Ataxia. **P.A. Lindahl***, J.D. Wofford

15:10 – 358. Thermal reaction of iron carbide particles produced by sonochemical synthesis. **Y. Yamada***, R. Miyatani, Y. Kobayashi

15:30 – 359. Relationship between structural and visible light activated photocatalytic ability of iron containing aluminosilicate glass. **Y. Iida**, S. Kubuki, K. Akiyama, H. Zoltán, K. Erno, K. Balazs, S. Katalin, T. Nishida

15:50 coffee break

16:00 – 360. Mössbauer study of the $\text{Fe}^{II}/\text{Fe}^{III}$ intermediates in PB/TiO_2 photo-Fenton system. X. Li, **J. Wang**, A. Rykov, V. Sharma, H. Wei, C. Jin, X. Liu, C. Sun, D. Dionysiou

16:20 – 361. Emission Mössbauer study on radioactive ^{57}Mn doped tin oxide films. **K. Nomura***, H. Gunnlaugsson, T.E. Melholt, S. Shayestehaminzadeh, K. Johnston, R. Mantovan, H. Masenda, M. Ncube, K. Bharuth-Ram, H.P. Gliserson, G. Langouche, D. Naidoo, S. Ölfansson, G. Weyer

16:40 – 362. Computational study on Mössbauer parameters for ^{151}Eu and ^{237}Np by means of scalar relativistic density functional theory. **M. Kaneko**, S. Miyashita, S. Nakashima

Hilton Hawaiian Village
Rainbow Tower, Rainbow 1

Metal-containing π-Conjugated Systems: Syntheses, Properties, Applications (#269)

Organized by: M. Humphrey, V. Yam, M. Akita

Presiding: G.A. Koutsantonis, W. Sun, V. Yam

13:00 – 363. Effects of the extended π -conjugation of diimine and cyclometalating ligands on the photophysics and reverse saturable absorption of heteroleptic cationic $\text{Ir}(\text{III})$ complexes. **W. Sun***

13:20 – 364. Study of charge transfer properties in metal containing block copolymer-carbon nanotube hybrid materials. H. Shi, L. Du, D.L. Phillips, **W. Chan***

13:40 – 365. Systematic studies to elucidate the role of metal ions in conducting metallocopolymers. M.T. Nguyen, **B.J. Holliday***

14:00 – 366. Platinum containing π -conjugated oligomers and polymers: Triplet excited states and applications. **K. Schanze**

14:20 – 367. Conjugated materials incorporating metal thiophenediethiolenes: Synthetic approaches to tuning electronic and optical properties. K. . Konkol, E.J. Uzelac, C. Amb, **S. Rasmussen**

14:40 – 368. Novel rhodacyclopentadienes – a new class of luminescent organometallics. **T. Marder***

15:00 Coffee break

15:15 – 369. Femtosecond Z-scan studies of nonlinear absorption and refraction of metal-containing molecules and nanostructures. **M. Samoc***

15:35 – 370. Functional metallocopolymers as precursors to magnetic metal alloy nanoparticles: Synthesis, lithographic patterning, and applications. **W. Wong***

15:55 – 371. Spectroscopic properties of a cholesteric liquid crystal glass platinum acetylde. **T.M. Cooper***, D. Krein, J. Haley, D. Stewart, S. Long, R. Ziolo, A. Glushchenko

16:15 – 372. Multinuclear sandwich complex containing extended π -conjugated unsaturated hydrocarbon ligands. **T. Murahashi***

16:35 – 373. Metal-polycyclic-aromatic-hydrocarbon emitters. **J. Yip***

16:55 Closing remarks

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2

Dioxygen Activation Chemistry of Metalloenzymes and Models (#339)

Organized by: A. Rosenzweig, S. Itoh, W. Nam

Presiding: S. Itoh

13:00 – 374. Proton-coupled electron transfer in catalysis by dioxygenases. **J. Roth***

13:30 – 375. New methods to activate dioxygen and generate and control the reactivity of high-valent metal-oxo porphyrinoid species. **D. Goldberg***, H. Neu, G. Baglia, J. Zaragoza, E. Joslin

14:00 – 376. Active intermediates generated in dioxygen activation and their reactivity relationships. **G. Yin***

14:30 – 377. Tuning Mn-peroxy O-O bond lengths, and the relative stability of dioxygen intermediates, via systematic ligand modification. **J. Kovacs***, M. Coggins, J. Rees, A. Johansen, M. Dedushko

15:00 – 378. Metal-oxo and metal-hydroxo species in biology. **A.S. Borovik**

15:30 – 379. Relationship of structure and reactivity of $\text{Ni}-\text{O}_2$ adducts. **J. Cho***

16:00 – 380. Intermolecular C-H activation by superoxide and chalcogenide nickel complexes. **C.G. Riordan***

16:30 – 381. Synthesis, characterization, and reactivity of high-valent transition metal-oxo complexes. **K. Ray**, C. Limberg, M. Driess

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

New Frontiers in Bioinorganic Chemistry (#356)

Organized by: M. Yamaguchi, S. Cohen, X. Ottenwaelder

Presiding: Y. Mikata, L.J. Wright

13:00 – 382. Inorganic radiopharmaceutical chemistry. **C. Orvig***

13:30 – 383. Photoinduced hydrogen evolution using $[\text{NiFe}]$ hydrogenase with phospholipid liposomes system. **H. Itó**, T. Iwasaki, I. Okura, T. Kamachi*

13:50 – 384. Efficient co-delivery of a Pt(IV) prodrug and a p53 activator to enhance the anticancer activity of cisplatin. **G. Zhou**

14:10 – 385. Molecular strategies targeting the iron metabolism of cancer cells. **E. Tomat***, E.A. Akam

14:30 – 386. Effect of iron ion on the specificity of photodynamic therapy using 5-aminolevulinic acid. **S. Ogura**,

M. Hayashi, H. Fukuhara, K. Inoue, T. Shuin, Y. Hagiya, M. Nakajima, T. Tanaka

14:50 Break

15:00 – 387. New metal-drug conjugates for treatment of parasitic diseases. **P. Chellan***, J. Davies, S.A. Ward, K.M. Land, P.J. Sadler

15:15 – 388. Bismuth(III) phosphinate complexes as antibacterial agents. **M. Werrett***, P. Andrews, R. Brarmananth, P. Crelin

15:35 – 389. Quinoline-based ligand design for fluorescent sensing of metal ions. **Y. Mikata***

15:55 – 390. Novel bio-luminogenic probes for continuous imaging of various biological phenomena in deep tissues of living animals. **Y. Urano***

16:25 – 391. Inorganic bridges between chemotherapy with biolumaging. **Z. Guo***

16:55 closing remarks

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

Isotope Production--Providing Important Materials for Research and Applications (#363)

Organized by: D. Phillips, K. Gagnon, Y. Hatsukawa

Presiding: K.M. Gagnon, S.E. Lapi

13:00 – 392. Production of alpha-emitting radioisotopes using the cyclotron facilities at Osaka University and JAEA Takasaki and the Tandem accelerator at Tokai, JAEA. **K. Washiyama***, R. Amano, E. Maeda, A. Yokoyama, I. Nishinaka, K. Hashimoto, S. Watanabe, N.S. Ishioka, N. Takahashi, A. Shinohara

13:25 – 393. Overview of the U.S. Department of Energy's effort to develop accelerator production of Ac-225. **K.D. John***, E. Birnbaum, R. Copping, D. Denton, J.W. Engle, M. Fassbender, M. Ferren, J. Fitzsimmons, D. Medvedev, S. Mirzadeh, J. Griswold, J. Krueger, K. Murphy, L. Mausner, V. Radchenko, W. Runde, D. Stracener, P. Pile, F.M. Nortier, D.R. Phillips

13:50 – 394. Isotopes for science and medicine: The pursuit, study, and application of theranostic isotopes at TRIUMF. **P. Schaffer**, J.R. Crawford, P. Kunz, H. Yang, R. Laxdal, L. Merminga, D. Wilbur, T. Ruth

14:15 – 395. Development of radiochemical separation of Ac isotopes from proton irradiated thorium target. **J. Fitzsimmons***, M. Fassbender, V. Radchenko, R. Copping, D. Denton, J.W. Engle, D. Medvedev, K. Murphy, J. Griswold, F.M. Nortier, E. Birnbaum, L. Mausner, S. Mirzadeh, K.D. John

14:35 – 396. Spectroscopic efforts to understand actinium behavior in solution. **M.G. Ferrier***, J.J. Wilson, V. Radchenko, S.A. Kozimor, J.W. Engle, K.D. John

14:55 Break

15:10 – 397. Isolation of At-211 using a solid phase anion exchange method. **S. Watanabe***, S. Watanabe, I. Sasaki, D. Wilbur, N.S. Ishioka, Y. Ohshima, D. Hamlin, C. Ming-Kuan, E. Balkin

15:30 – 398. Development of a novel lanthanide and actinide separation method utilizing solid electrolytes. **K.G. Myhra***, M. Du

15:50 – 399. Harvesting of long-lived radioisotopes from an aqueous target at the National Superconducting Cyclotron Laboratory. **G.F. Peaslee***, A. Pen, B. Marois, N. Hubley, T. Mastren, S. Loveless, E. Bollinger, S.E. Lapi, D.J. Morrissey

16:15 – 400. Production of ^{119}Te from proton-irradiated ^{nat}Sb for generators of ^{119}Sb . **J.W. Engle***, V. Radchenko, J.J. Wilson, M.A. Mosby, P. Ellison, T.E. Barnhart, R.K. Nickles, M. Fassbender, S.A. Kozimor, K.D. John, E. Birnbaum, F.M. Nortier

16:35 – 401. Development of a pilot scale facility for production of enriched stable isotopes. **K.J. Hart**, B. Eggle, B. Stevenson, W. Strunk, G. Giles

Wednesday Evening

Hawaii Convention Center
Halls I, II, III

Lewis Acid/Base Pair Chemistry in Molecular Transformations, Catalysis and Energy Storage (#65)

Organized by: T. Autrey, D. Stephan, z. Wang

Presiding: T. Autrey, D. Stephan, Z. Wang

Poster Session

19:00 – 21:00

402. Geminal Al/P-based frustrated Lewis-pair in molecular activation. **P. Wegener***, W. Uhl

403. FLP's as dehydrogenation catalysts: Research in an undergraduate inorganic laboratory course. **G.M. Edvenson***, C.B. Anderson, K. Gurung, B.A. Isaacson, S. Janakan, K.M. Jensen, C.W. O'Keefe, A. Rahimi, J.A. Rumrich

404. Solid phase frustrated Lewis pairs for small molecule activation. **J. Xing***, J. Buffet, D. O'Hare

405. Revival of frustrated Lewis pairs from shelf-stable complexes comprised of borane and N-phosphine oxide substituted imidazolidine. **T. Kinoshita**, Y. Hoshimoto*, M. Ohashi, S. Ogoshi*

406. Effect of preparation method on 1,2-dichloropropene combustion with $\text{Fe}_2\text{O}_3/\text{WO}_x\text{-ZrO}_2$. **Y. Shinada***, N. Ikenaga

407. Reactivity of a Ga/P-based frustrated Lewis pair. **J. Possart***, W. Uhl

408. Planar N-heterocyclic carbene-boron ion based Lewis acid catalysis. **L. Cao**

409. Main group Lewis-acid catalyzed hydrothiolation of alkenes. **E. Mosaferi***, M. Perez, D. Stephan

410. Controlling the Lewis acidity of boranes: Balancing front- and back-strain. **E. Dorkó***, H. Mehdi, T. Soós

411. Reduction of ketones and aldehydes with moisture tolerant FLP catalyst. **M. Bakos***, Á. Gyömöre, I. Papai, T. Soós

412. Metal-free frustrated Lewis pair hydrogenation catalysis. **E.N. Daley**, D. Stephan

413. Oxidation reactions and C-O bond cleavage catalyzed by organorhenium oxides. **B. Zhang**, C. Li, F. Kuhn, T. Zhang

* Principle Author

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Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Nuclear Probes in Nanoscale Characterization (#254)

Organized by: M. Takahashi, A. Hill, V. Sharma, J. Wang, M. Takahashi, M. Takahashi, K. Nomura, Y. Yamada Presiding: K. Nomura, M. Takahashi

19:00 – 414. In-beam Mössbauer spectra of ^{57}Mn implanted in mixed mixtures of CH_4 and Ar. S. Tanigawa, **Y. Kobayashi**, Y. Yamada, M.K. Kubo, M. Miura, W. Sato, J. Miyazaki, Y. Sato, D. Natori, S. Sato, A. Kitagawa

19:05 – 415. Time-resolved In-beam Mössbauer spectra obtained after ^{57}Mn implantation in LiH and LiD. **Y. Sato**, Y. Kobayashi, Y. Yamada, M.K. Kubo, M. Miura, T. Nagatomo, J. Miyazaki, W. Sato, S. Tanigawa, D. Natori, S. Sato, A. Kitagawa

19:10 – 416. Emission Mössbauer study on radioactive ^{57}Mn doped In_2O_3 films. **K. Nomura***, A. Mokhles Gerami, H.P. Gunnlaugsson, T.E. Molholt, K. Johnston, R. Mantovan, H. Masenda, Y. Matveyev, V.N. Adoos, M. Ncube, S. Shayestehaminzadeh, I.U. Solozabal, K. Bharuth-Ram, H.P. Gislaslon, P.B. Krastev, G. Langouche, D. Naidoo, S. Ölafsson, G. Weyer, A. Zenkevich

19:15 – 417. Structure investigation of Fe substituted Ni-Si intermetallics as hydridesulfurization catalysts. **C. Liang**

19:20 – 418. Mössbauer study of iron (III) sulfide particles produced by a polyol method. **I. Kubono***, Y. Yamada, Y. Kobayashi

19:25 – 419. Mössbauer study of iron carbide nanoparticles produced by laser ablation in organic solvents. **S. Amagasa***, Y. Yamada, Y. Kobayashi

19:30 – 420. Formation of rock-salt structured iron nitride thin films using pulsed laser deposition. **M. Sato**, Y. Yamada, Y. Kobayashi

19:35 – 421. Formation process of oxygen vacancy in ZnO studied by perturbed angular correlation method. **S. Komatsuda***, W. Sato, Y. Ohkubo

19:40 – 422. Development of dilute magnetic materials - magnetic property and Mössbauer spectra of SrSnO_3 doped with Fe and Sb. **S. Suzuki***, Y. Koike, K. Nomura, A. Okazawa, N. Kojima

19:45 – 423. New type of cationic ordering in Prussian Blues. A. Rykov, X. Li, K. Nomura, **J. Wang**

19:50 – 424. Mössbauer spectra of organo-atrmin(V) complexes having Sb–Au bond. **M. Takahashi***, S. Ohno, S. Matsukawa

19:55 Discussion

Hawaii Convention Center
Halls I, II, III

Dioxygen Activation Chemistry of Metalloenzymes and Models (#339)

Organized by: A. Rosenzweig, S. Itoh, W. Nam

Poster Session
19:00 – 21:00

425. Copper active-oxygen complexes generated by using N_3 -tridentate ligands bearing cyclic-diamine moiety with 2-(2-pyridyl)alkyl sidearm. **T. Abe**, Y. Morimoto, H. Sugimoto, N. Fujieda, S. Itoh

426. Biomimetic model studies on dicopper peroxy species using a pre-organized ligand. **Y. Funahashi**, K. NAGATA, T. Hatanaka

427. Aerobic alkane oxidation catalysis of iron and cobalt complexes with scorpionate ligands. **Y. Hayashi**, J. Nakazawa, S. Hikichi*

428. Construction of non-heme iron oxyge-nases-mimicking active sites on mesoporous silica supports. **S. Hikichi**, J. Nakazawa

429. Electrochemical properties of iron bispidine catalysts. S. Auras, P. Comba*, **M. Kerscher**, A. Waleska

430. Structure variations of transition metal complexes with $\text{N,N}'$ -(ethylene-di-p-phenylene)bis(pyridine-2-carboxamide) li-gand and their catecholase activities. **O. Kim**, h Lee*, S. Sarkar

431. Iron-catalyzed aerobic oxidation of primary aliphatic alcohols to carboxylic acids. **K.I. Lagerblom***, T. Repo

432. Electrochemical and spectroscopic studies of Cu-nitrosoarene complexes. **Y. LE MEST**, M.S. Askari, L. Wojcik, N. Le Poul, X. Ottenwaelder

433. New dinuclear models of galactose oxidase: Electrochemical and spectroscopic studies. F. Gennarini, I. Lopez, C. Belle, H. Janet, R. David, M. Réglier, **Y. LE MEST***, N. Le Pou

434. Quinone formation on the Tyr98 residue of the caddie protein correlative to the catalytic mechanism of tyrosinase. **Y. Matoba***, S. Kihara, N. Bando, M. Sakaguchi, K. Kayama, T. Kumagai, T. OGURA, M. Sugiyama

435. Hydroxylation of aromatic compounds with hydrogen peroxide catalyzed by Ni-complexes supported by pyridylalkyl-amino ligands. **Y. Morimoto***, S. Bunn, Y. takagi, S. Itoh

436. Ligand influence on superoxide dismu-tation by model Ni-complexes. **A. Mukherjee**, N. Singh, V. Snider

437. Synthesis and spectroscopic character-ization of a cryptate complex of tricoper-peroxo as a biomimetic model of multicopper oxidase. **K. NAGATA***, T. Hatanaka, T. Inomata, T. Ozawa, H. Masuda, Y. Funahashi

438. Characterization of mononuclear non-heme iron(III) superoxo and hydroperoxy complexes with N5 donor set. **J. Nakazawa***, F. Oddon, S. Hikichi*

439. Characterization of mononuclear non-heme cobalt(III) dioxygen complexes with N5 donor sets. **T. Nishiura***, J. Nakazawa, S. Hikichi

440. Reactivity of nickel-acylperoxo com-plexes. **F. Oddon***, J. Nakazawa, S. Hikichi

441. Development of homogeneous and het-erogeneous nickel complex catalysts based on triazolyl-BOX ligands and their catalytic activities toward alkane oxida-tion with mCPBA. **K. Sakamoto**, J. Nakazawa, S. Hikichi*

442. Mutations at the potential electron do-nors located in the outer coordination sphere of the trinuclear copper center in Cu_3O . **T. Sakurai***, K. Kataoka, M. Yamamoto

443. Dioxygen activation in human in-doelamine 2,3-dioxygenase isoform-1 ($\text{hIDO}1$): Uncovering the mechanism of catalytic O–O bond cleavage that avoids enzyme deactivation. I.M. Chrisman, L.S. Dameron, **V.V. Smirnov***

444. Development of multi-functionalized poly(oxazolinyl)borate ligands and char-acterization of their nickel(II) complexes. **K. Takamura***, S. Hikichi, J. Nakazawa

445. Photochemical reactivity of cyclometa-lating iridium(III) complexes with fla-vonols. **A. Takura**, K. Ohno, A. Nagasawa, T. Fujihara

446. Alkane oxygenation catalysis of nickel complexes with oxazoline-based biden-tate and tridentate ligands. **I. Takashi***, J. Nakazawa, S. Hikichi

447. Four-electron reduction of dioxygen catalyzed by dinuclear cobalt complex. **M. Wada**, Y. Miyazato, T. Wada

Hawaii Convention Center
Halls I, II, III

Isotope Production--Providing Important Materials for Research and Applications (#363)

Organized by: D. Phillips, K. Gagnon, Y. Hatsukawa

Poster Session

19:00 – 21:00

448. Production of radiochemically pure Ho-163 sources for the ECHO experiment. **C.E. Duellmann***, K. Chrysaldis, T. Day Goodacre, H. Dorrer, K. Eberhardt, C. Enss, L. Gastaldo, R. Haas, C. Hassel, K. Johnston, T. Kieck, U. Köster, B. Marsh, C. Mokry, S. Rothe, J. Runke, F. Schneider, T. Stora, A. Türler, K. Wendt, f. the ECHO collaboration

449. Improvement in production yield of ^{85}Sr at C_60 using nuclear recoil. **Y. Miyashita**, K. Akiyama, Y. Hatsukawa, S. Kubuki

450. Molecular laser isotope separation without tunable lasers: Isotope-selective ion-ization of N_2 isotopologues using femto-second laser-induced molecular alignment. **H. Akagi**, T. Kasajima, T. Kumada, R. Itakura, A. Yokoyama, H. Hasegawa, Y. Ohshima

451. Measurement of alpha-induced reac-tion cross sections of Cr isotopes on nat-ural Ti. **H. Kikunaga***, M. Murakami, Y. Komori, H. Haba

452. High-activity fission fragment sources: Challenges of producing sources for CARIBU. **J. Burns**, S.M. Van Cleve, N.J. Sims, E.H. Smith, D. Stracener, R. Boll

453. Isotope fractionation in AgI super – ionic conductor by centrifugation. **M. Ono***, S. Okuyasu, Y. Iguchi, F. Esaka, E. Ishitsuka, T. Osawa, Y. Ogata, T. Mashimo

454. Kinetic study of hydrogen isotope effect on hydrogen electrode reactions. **S. Shibuya**, H. Matsushima, M. Ueda

455. Metallofullerene encapsulating artificial radio element of Pm. **S. Miyachi**, K. Akiyama, H. Kikunaga, S. Kubuki

Thursday Morning

Hawaii Convention Center
Halls I, II, III

Organo-Main Group Avenues toward Advanced Materials (#16)

Organized by: T. Baumgartner, S. Liu, S. Yamaguchi

Poster Session

10:00 – 12:00

456. BN-acenes: Synthesis, reactivity, and optoelectronic properties. **J.S. Ishibashi**, S. Liu

457. Electrophilic borylation for the synthesis of B,N containing poly aromatic hydro-carbons. **A. Escande**, M.J. Ingleson*

458. Toward highly conjugated materials: The quest for polyazaborinines. **S.K. Mellerup**, S. Wang

459. Synthesis of boron- and nitrogen-con-taining conjugated systems by reaction of bis(silyl)pyrazines with haloboranes. **M. Noguchi**, T. Yurino, H. Tsurugi, K. Mashima, K. Suzuki, M. Yamashita*

460. Basicity of non-solvated boryl anion: Deprotonation of benzene. **T. Osato**, Y. Okuno, S. Ishida, T. Iwamoto, M. Yamashita*, K. Nozaki*

461. Synthesis and reactivity of neutral di-boranes – the alkene analogs. **S. Ullrich**, H. Braunschweig*

462. Synthesis, structure, and reactivity of the first isolable diarylboron ion. **N. Tanaka**, Y. Shoji, T. Fukushima*

463. Reactivity of (*tert*-butylimino)mesitylbo-rane. **M. Schäfer***, H. Braunschweig

464. Diboron chelate complex with oxalyl pyrrolidine as a new electron-accepting unit. **H. Shimogawa**, A. Wakamiya*, Y. Murata*

465. Fluorescent main-chain and side-chain polymers derived from boron difluoride formazanate complexes. **S.M. Barbon**, S. Novoa, R.R. Maar, J.A. Paquette, J.B. Gilroy*

466. Synthesis and properties of triarylbo-rane Lewis acids with phosphine oxide groups. **M. Park***, J. Kwak, N.V. Nghia, M. Lee*

467. Highly efficient organic light emitting diodes using donor-acceptor type triaryl-boron compounds showing thermally ac-tivated delayed fluorescence. **K. Suzuki**, S. Kubo, K. Shizu, A. Wakamiya, T. Fukushima, Y. Murata, C. Adachi, H. Kaji*

468. Synthesis and properties of alumina-and galla-benzenes. **T. Nakamura**, K. Suzuki*, M. Yamashita*

469. Indium complexes with pendatate di-nucleating ligands for poly(lactic acid) po-lymerization. **A. Kremer**

470. Cationic chiral indium complexes and their reactivity in polymerization of func-tionalized monomers. **C. Chang***, P. Mehrkhodavandi

471. Small molecule activation under mild conditions by main group metal clusters. **P. Vasko**, H.M. Tuononen, P.P. Power*

472. Band edge control of crystalline silicon by chemical functionalization of the sur-face. **N.T. Plymale**, A.A. Ramachandran, A.N. Lim, B.S. Brunschwig, N.S. Lewis*

473. Synthesis, properties, and reactions of quinone-fused siloles. **K. Sakamoto***, T. Kawasaki, C. Kawabe, T. Watanabe

474. Bright solid-state emission in disilane-bridged arenes including donor and acceptor moieties. **M. Shimada**, R. Sakamoto, Y. Yamanoi, H. Nishihara*

475. Theoretical calculation and synthtic study on Si-bridged π -conjugated sys-tems. **E. Ohta**, T. Ogaki, T. Aoki, Y. Oda, Y. Matsui, H. Ikeda*

476. Synthesis of 1,4-naphthalenediy-bridged molecular gyrotops and cage-size effects on dynamics in solution. **Y. Nishiyama**, A. Koyama, Y. Inagaki, K. Yamaguchi, W. Setaka*

477. Synthesis of a dimeric silylene tungsten complex and its dissociation equilibrium with a monomer in solution. **T. Yoshimoto**, H. Hashimoto, N. Hayakawa, T. Matsuo, H. Tobita*

478. Palladium and platinum complexes of an isolable dialkyldisilyne. **S. Ishida***, Y. Misawa, T. Iwamoto*

479. Transformation of azulenes using an isolable dialkylsilylene. **T. Kosai**, S. Ishida, T. Iwamoto*

480. Cationic donor-acceptor complexes of group 14 elements in multiple oxidation states. **P.A. Gray**, N. Burford*, B. Patrick

481. Preparation and reactions of oxygen-functionalized dibenzodisilacyclohexa-diene. **T. Kawasaki**, K. Sakamoto*

482. Preparation and reactions of 1-cy-clobutylsilsilanes. **T. Sugino**, K. Sakamoto*

483. Synthesis, properties, and reactions of oligoisletanes. **W. Yang**, K. Sakamoto*

484. Synthesis of a novel molecular gear having a germanium junction and its gear slippage. **K. Okamura**, Y. Inagaki, K. Yamaguchi, W. Setaka*

485. Molecular gyrotop with germanium junctions: Dynamics of a phenylene rotor in a crystalline state. **Y. Inagaki**, K. Yamaguchi, W. Setaka*

486. Phosphoviologens: Powerful electron-acceptors with tunable optical and elec-tronic properties. **M. Stolar**, C. Reus, T. Baumgartner*

487. Synthesis and physicochemical prop-erties of phosphorus analogs of phthalimides and naphthalimides. **K. Hatanaka**, Y. Takeda, S. Minakata*

*** Principle Author**

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onlineprogram

- 488.** Triphosphasumanenes: A Janus-type π -surface. **S. Furukawa***, Y. Suda, J. Kobayashi, T. Kawashima, M. Saito
489. Synthesis, structure, photophysical property, and one-electron reduction of boryl-substituted diphosphene. **S. Asami**, M. Okamoto, K. Suzuki, M. Yamashita*
490. Synthesis of phospha-, stiba-, and bis-mutha-benzenes via metathensation of the 2,5-bis(silyl)-1-alumina-2,4-cyclohexadiene. **T. Ishii**, T. Nakamura, K. Suzuki*, M. Yamashita*
491. Structures and electronic states of hydride-antimony compounds having Sb-Au bond. **S. Ohno**, M. Takahashi, S. Matsukawa
492. Preparation and some reactions of trithiocyclododecatriene. **S. Oka**, K. Sakamoto*
493. Reactions of di-*t*-butylcyclopropane with Peterson and Wittig reagents. **K. Hanitani**, K. Sakamoto*
494. Synthesis of compounds bearing ferrocenyliothiocarbonyl groups toward functional dyes. **H. Miyake***, T. Tajima, Y. Takaguchi
495. Synthesis and development of 1,2,4,6-thiatriazinyl and 1,2,4,6-selenatriazinyl π -radicals for applications in molecular electronics. **N. Uttronkie**, A. Leitch, J. Klein, I. Korobkov, J. Brusso*
496. 1,1-Carboration as a facile route to tellurium–boron heterocycles. **F. Tsao**, D. Stephan
497. Reactivity and photochemistry at the tellurium center of π -conjugated tellurophenes. **E.I. Carrera**, T.M. McCormick, M.J. Kapp, A.J. Lough, D.S. Seferos*

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Functional Nanomaterials Based on Coordination Chemistry (#73)

- Organized by:* T. Uemura,
M. MacLachlan, H. Matsui
Presiding: T. Uemura
- 8:00** Opening remarks
8:05 – 498. Crystalline sponge method updated. **M. Fujita***
8:30 – 499. Exploring the synthesis and solid state behavior of coordination polymers and complexes. **J. Martí-Rujas***
8:50 – 500. Dynamic metal-organic polyhedra. **S. Kang**, K. Hamachi, S. Kanegawa, O. Sato
9:05 – 501. Directing the assemblies of organic donor-acceptor type chromophores within metal-organic frameworks for improved luminescence. **J.K. Klosterman**
9:20 – 502. Variation in porous coordination polymer structure due to deprotonation level of hydroxyl groups of a flexible bi-functional linker. A.A. Bezrukova, K.W. Törnroos, **P.D. Dietzel**
9:35 – 503. Discrete cyclic supramolecules and nanotubes self-assembled to form porous materials. **A. Comotti**, S. Bracco, L. Marchio', A. Ienco, P. Sozzani
9:55 Break
10:05 – 504. Polyaromatic coordination capsules displaying unique host-guest behavior. **M. Yoshizawa***
10:25 – 505. Metal-directed assembly of discrete coordination cage. **F. Li**
10:40 – 506. Chemical systems and materials using subcomponent self-assembly. **J.R. Nitschke**
11:00 – 507. Controlling the electronic states and physical properties of semiconducting MX- and MMX-type chain complexes. **H. Iguchi***, M.R. Mian, S. Takaishi, M. Yamashita
11:15 – 508. New strategy for designing silver(I) coordination complexes for olefin/paraffin separations. **M.G. Cowan**, W. McDanel, H.H. Funke, Y. Kohno, D. Gin, R.D. Noble
11:30 – 509. Photoresponsive materials using metal-ion coordination. **A.D. Ostrowski***

- 11:45 – 510.** Highly efficient incarceration and selective extraction of inorganic anions from water by self-assembled nano-jars. **G. Mezei***

Hawaii Convention Center
Halls I, II, III

Molecular Catalysis of Water Splitting Reactions (#76)

Organized by: K. Sakai, L. Sun, G. Brudvig, L. Spiccia

Poster Session

10:00 – 12:00

- 511.** Unravelling the mechanism of water oxidation catalysed by novel tacl-based ruthenium complexes. **C. Casadevall***, D. Lloret Fillo, D. Costas

- 512.** Molecular photo-charge-separators enabling single-pigment-driven multi-electron storage leading to catalytic hydrogen evolution. **K. Kitamoto**, K. Sakai*

- 513.** Development of novel penta-nuclear hetero-metal clusters and their electrochemical properties. **H. Izu**, M. Okamura, R. Kuga, P. Vijayendran, N. Katsuta, S. Kawata, M. Kondo, S. Masaoka*

- 514.** Studies on electrochemical hydrogen evolution from water catalyzed by bis(dithiolato)nickelate(II) complexes.

- K. Koshiba**, K. Yamauchi*, M. Huynh, S. Hammes-Schiffer, K. Sakai*

- 515.** Construction of new water oxidation catalyst with a pyrophosphate-bridged Ru(III, IV) framework. **Y. Miyazato***, T. Wada

- 516.** Photocatalytic hydrogen evolution from water catalyzed by cobalt-NHC complexes under low driving forces. **K. Kawano**, K. Yamauchi*, K. Sakai*

- 517.** Water oxidation catalyzed by the dinuclear ruthenium complex bridged by bis(terpyridyl)anthraquinone. **S. Nishimura**, T. Wada*, Y. Miyazato

- 518.** Hydrogen evolution from water catalyzed by nickel(II) pyridinethiolate complexes having oligopeptide residues. **K. Miyazaki**, K. Kitamoto, K. Yamauchi, K. Sakai*

- 519.** Dinuclear acetato-bridged palladium(II) complexes for photoreductive production of hydrogen. **T. Kitamura***, Y. Kataoka, T. Kawamoto

- 520.** Development of molecular catalysts for hydrogen evolution using a one-step two-electron reduction scheme. **S. Nakashima**, K. Yamauchi*, K. Sakai*

- 521.** Water oxidation reaction catalyzed by a pentanuclear iron complex. **M. Okamura**, M. Kondo, R. Kuga, S. Hayami, M. Yoshida, K. Yoneda, S. Kawata, S. Masaoka*

- 522.** Tandem photocatalysis as a strategy for water splitting. **N. Alderman***, J. Sommers, C.J. Viasus, **S. Gambarotta**

- 523.** Improving stability during photoinduced water oxidation catalysis by cobalt porphyrins. **T. Nakazono**, A.R. Parent, K. Sakai*

- 524.** Study of water splitting at the Mo-Cu center of carbon monoxide dehydrogenase using realistic in silico models. **D. Rokhsana***, T. Large, M. Dienst, M. Retegan, F. Neese

- 525.** Photocatalytic hydrogen evolution from water catalyzed by Pt(II)-based molecular catalysts encapsulated with a supramolecular cage. **S. Tanaka**, T. Nakazono, K. Yamauchi, K. Sakai*

- 526.** Enhancing electrocatalytic hydrogen evolution by nickel molecular catalysts with the aid of Lewis acids in aqueous media. **H. Shao**, H. Soo

- 527.** Photochemical water oxidation catalyzed by a water soluble copper phthalocyanine derivative. **R. Terao**, T. Nakazono, A.R. Parent, K. Sakai*

- 528.** Hydrogen production from water under visible light using tetranuclear metal (Pd and Ni) complexes. **Y. Yan**, T. Kawamoto

- 529.** Kinetic studies of Pt(II)-catalyzed H₂ evolution revealing the formation of diplatinum intermediates. **F. Wakiyama**, K. Yamauchi*, K. Sakai*

- 530.** Synthesis of multinuclear manganese complexes having a cage-type ligand: Structural models of oxygen evolving center. **S. Yonaga**, K. TANGE, T. Hatanaka, Y. Funahashi*

- 531.** Z-scheme photosynthesis for H₂ evolution from water forming a three-electron-reduced species. **K. Yamamoto**, K. Kitamoto, K. Sakai*

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Coordination and Supramolecular Chemistry for Aqueous Metal Ion Separations (#97)

Organized by: R. Ellis, D. Robinson, R. Motokaza

- 8:00 – 532.** New highlights on niobium and tantalum chemistry in alkaline media. **V. Weigel**, G. Delobelle*, G. Cote, S. Bélaïr, A. Chagnes

- 8:25 – 533.** Assessing the effects of new reagents for iron control in medium temperature sulphide concentrate leaching. **E. Asselin**, B. Abdul

- 8:50 – 534.** Thermodynamic study of uranium peroxide and oxalate neodymium precipitations. **M. Bertrand***, S. Lallemand, E. Plasari, F. Auger, p. moiisy

- 9:15 – 535.** Polyoxythiomolate chain of unprecedented [Mo₁₇O₆₈Sg]¹⁸⁻ clusters. **Y. Yu**, H. Wang*, C. Zhao, Z. Zhang, H. Ma*, H. Pang*

- 9:40 – 536.** Recycling processes of lithium-ion batteries. **A. Chagnes***, G. Cote

10:05 Break

- 10:20 – 537.** Solvent extraction separations using CYANEX® 572. **M.D. Soderstrom***, T. McCallum, A. Quildron

- 10:45 – 538.** Cutting the fat - using model systems to probe metal ion-extractant interactions. **M.I. Ogden**, K.R. Barnard

- 11:10 – 539.** Extraction of the rare earth elements from neodymium manganite leachate via solvent extraction using non-phosphorous organic extractants (amides derivatives). **M. Gergorić**, M. Tyumentsev, T. Retegan, C. Ekberg, B. Steenari

- 11:35 – 540.** Fundamental investigation of structure of neodymium-di-(2-ethylhexyl) phosphoric acid combinations usinf ESI and MALDI spectrometry and NMR spectroscopy. **C. Scharf***

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Frontiers of Molecular Magnetism (#109)

Organized by: H. Oshio, J. Miller, R. Oakley, S. Brooker, S. Gao, M. Ohba
Presiding: G. Christou, H. Oshio

8:00 Opening Remarks

- 8:05 – 541.** New homo- and heterometallic single-molecule magnets and related clusters. **G. Christou**

- 8:35 – 542.** Symmetry strategy to enhance the magnetic anisotropy of single-molecule magnets. **J. Liu**, Y. Chen, J. Liu, L. Ungur, L. Chibotaru, M. Tong

- 8:55 – 543.** New polynuclear metal complexes with unprecedented structural motifs and single-molecule magnetic behaviors. **P. Perlepe, D. Alexopoulos, J. Tang, G. Christou, T. Stamatatos***

- 9:15 – 544.** Magnetically interesting coordination complexes of macrocyclic ligands - from single ion magnets to MRI contrast agents. **M. Pilkington***

- 9:35 – 545.** Molecule-based quantum magnets composed of poly-HF ligands. **J.L. Manson***

9:55 Break

- 10:10 – 546.** New trends and advances in single-molecule magnets. **M. Murugesu***

- 10:30 – 547.** We can get higher spins and higher anisotropy but how can we get higher blocking temperatures for SMMs?. **A. Powell***

- 10:50 – 548.** SMM behaviors of isostructural Zn(II)-Ln(III)-Zn(II) tri-nuclear complexes (Ln = Ce, Nd, Tb, and Dy). **T. Kajiwara**, C. Takehara, P. Then, Y. Kataoka

- 11:10 – 549.** Molecular magnets based on a modular approach. **K.R. Dunbar**
11:30 – 550. Lanthanide single-molecule magnets: Design and relaxation dynamics. **J. Tang***

Hawaii Convention Center
Halls I, II, III

Frontiers of Organo-f-element Chemistry (#125)

Organized by: F. Edelmann, P. Diaconescu, Y. Chen, D. Emslie, P. Junk

Poster Session

10:00 – 12:00

- 551.** Direct allylation of benzylic alcohols with allylsilanes catalyzed by Sc(OTf)₃. **Y. Di***, Y. Kimura, A. Toshimitsu, T. Kondo*

- 552.** Tris(pyrazolyl)borate-supported lanthanide(III) amide-halide complexes. **R. Thim**, C. Maicle-Mössmer, R. Anwander

- 553.** Rare earth metal-mediated group transfer polymerization of vinylphosphonates: Tuning the metal ligand interaction via steric crowding at the rare earth center and novel highly efficient initiators from C-H bond activation. **B.S. Soller***, B. Rieger

- 554.** Molecular structure and luminescence of a series lanthanide complexes with helical structures. **M. Hasegawa***, A. Ishii

- 555.** Toward C-H activation of hydrocarbons by rare earth NHC-complexes. **J. Rieb***, P.L. Arnold, F. Kuhn

- 556.** Exploring a new coordination mode of f-elements: Ln(III) complexation with nitrogen-phosphorus donor ligands. **Z. Zhang**, X. Li, P. Zanonato, P.D. Bernardo, L. Rao

- 557.** Advances in tris(amide) uranium chemistry: Work toward generating U=P bonds. **B.C. Stobbe**, R.K. Thomson*

- 558.** Cerium-catalyzed aerobic oxidation of arylmethanols under dioxygen atmosphere. **H. Tsurugi***, M. Paul, S. Shirase, L. Mathey, M. Balasubramanian, S. Tanaka, K. Mashima*

- 559.** Synthesis and characterization of high symmetry phosphinimide-acnide complexes. **S.B. Younger-Mertz**, R.K. Thomson

- 560.** Assessing single-molecule magnet and luminescent properties of ferrocene di-amide rare earth complexes. **J.L. Brosmer***, W. Huang, P.L. Diaconescu

Hawaii Convention Center
Halls I, II, III

Electron Transfer and Electrochemistry of Inorganic and Organometallic Materials (#126)

Organized by: H. Nishihara, P. Harvey, W. Wong
Presiding: P.D. Harvey, H. Nishihara, W. Wong

Poster Session

10:00 – 12:00

- 561.** Synthesis and characterization of new late transition metal(II) thiosemicarbazone complexes. **N. Arefyeva***, A. Klein

* Principle Author

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- 562.** Synthesis and carrier transport properties of semiconducting materials consisting of HAT derivatives and copper halides. **K. Himoto**, T. Okubo*, M. Maekawa, T. Kuroda-Sowa
- 563.** Syntheses and physical properties of 1D halogen-bridged metal complexes by using hydroxyl functional groups. **M.R. Mian***, H. Iguchi, S. Takaishi, M. Yamashita
- 564.** Electrochemical behavior of the Ni-mixed Prussian-blue analog spin-coated thin film. **M. Ishizaki**, K. Ono, K. Kanaiwa, M. Kurihara
- 565.** Fabrication of oriented Prussian-blue nanocrystalline thin films and their electrochemical properties. **K. Ono**, M. Ishizaki, K. Kanaiwa, M. Kurihara*
- 566.** Development of thin film solar cells of d- π complexes using HATNA-Cl₆. **Y. Kono**, K. Himoto, K. Nakatani, K. Tanishima, T. Okubo*, M. Maekawa, T. Kuroda-Sowa
- 567.** High performance zinc tin oxide thin-film transistor through dielectric interface effect. **K. Lim**, E. Lee, J. Ko, Y. Kim, N. Cho, C. Jo, J. Park, Y. Kim*
- 568.** Synthesis of nanoparticles of a copper coordination polymer with octamethylene ditiocarbamate and application to organic photovoltaics. **K. Nakatani**, T. Okubo*, M. Maekawa, T. Kuroda-Sowa
- 569.** Crystal structures and conducting properties of 3D coordination polymers with dithiocarbamate derivatives. **K. Tanishima**, T. Okubo*, M. Maekawa, T. Kuroda-Sowa
- 570.** Investigations on the mechanism of the catalytic conversion of nitrite to nitric oxide by a ruthenium nitrosyl complex. **J.H. Jordaan**, K.M. Miranda
- 571.** Synthesis and analysis of new graphic carbon nitride analogs. **S. Okamura**, T. Togashi, K. Kanaiwa, M. Kurihara*
- 572.** Synthesis of LiMnPO₄ by the microwave heating method. **T. Naka**, M. Sato, M. Higuchi*, K. Katayama
- 573.** Electrochemical properties of [M-7M] type nonanuclear clusters derived by asymmetric multidentate ligands. **Y. Tsuji***, T. Togo, A. Mishima, T. Koshiyama, M. Ohba
- 574.** Charge-transfer phase transition, phase separation, and visualization of local electronic states in a Pd-Br chain complex. **T. Yoshida***, S. Takaishi, H. Iguchi, M. Yamashita
- 575.** Multistep electrochromic behavior of an acetamidato-bridged dinuclear platinum complex bearing a cyclometalating ligand. **M. Yoshida**, N. Yashiro, H. Shitama, A. Kobayashi, M. Kato*
- 576.** C^NA^C cyclometallated platinum(II) complexes and their electrochemical behavior. **S. Garbe***, A. Klein
- 577.** Cyclometalated Ni(II) complexes carrying anionic tridentate C, N, N-ligands and varying coligands – synthesis and spectroelectro-chemistry. **N. Vogt***, A. Klein
- 578.** Cyclometallated Ni(II) complexes of the type [(R-PPh₂)NiBr] – synthesis and electrochemical studies. **A. Sandleben***, A. Klein
- Hawaii Convention Center
Halls I, II, III
- Non-covalent Interactions in Coordination Systems (#161)**
- Organized by: T. Konno, K. Lu, A. Hor
Presiding: T. Konno, N. Kuwamura, N. Yoshinari
- Poster Session**
10:00 – 12:00
- 579.** New transition metal complexes of ferrocene-bridged bisimine ligands with examples of rare Fe-M interactions. **K. Jess**, A.R. Petrov, M. Freytag, D. Baabe, T. Bannenberg, P. Jones, M. Tam*
- 580.** Structural characterization of ferrocene-dipeptide conjugates bearing pyridine oxide moiety. T. Moriochi, **H. Wu**, T. Hirao
- 581.** Pseudo crystal polymorphism of halogen-substituted tetraaza[14] annulene complexes. **N. Inaba***, S. Ichimura, M. Saeki, Y. Tamaki, K. Miyamura
- 582.** Crystal structure analysis of alkyl quaternary ammonium-[Ni(dmit)₂] complex salts bearing terminal cyclohexyl group. **S. Kakihara***, M. Saeki, S. Ichimura, Y. Tamaki, K. Miyamura
- 583.** Structural change process in single crystal of bis(diphenylglyoximate)nickel(II)-based complexes by alkoxy chain elongation. **K. Uejii***, S. Ichimura, K. Tomono, Y. Tamaki, K. Miyamura
- 584.** Synthetic and structural comparisons between group 14 dithiolato metathylenes and first row transition metal dithiolato complexes. **J.K. Pratt**, P.P. Power
- 585.** Ruthenium complexes bearing tridentate polypryldil with noncoordinating donor atoms: Construction of specific coordination space involving non-covalent interactions. D. Oyama*, T. Yamanaka, R. Tokoyoda, R. Abe*, T. Takase
- 586.** Synthesis and characterization of a pyrophosphate-bridged dinuclear ruthe- nium complex with 1,4,7-triethyl-1,4,7-triazacyclononane. **H. Tokinobu**, Y. Miyazato, T. Wada*
- 587.** Synthesis and electronic structure of dirhodium(II,II) complex with benzamidinato as bridging ligand. **S. Mikami***, Y. Kataoka, T. Kawamoto, T. Ikeue, M. Handa
- 588.** Synthesis and structures of platinum(II) complexes containing 8-(dimethyl or diphenylphosphino)quinoline. **M. Mori**, T. Suzuki, Y. Sunatsuki
- 589.** Synthesis and characterization of novel salicylaldimine – or naphthalimine-de- rivative ligands and their metal complexes. **N. Beynek**, N. Tan, H. Beynek
- 590.** Effect of an amino group on electro- chemical properties of di- and mononu- clear iron complexes with N, C-S-triden- tate ligands. **T. Nakae**, M. Hirotsu*, I. Kinoshita
- 591.** Redox properties and catalytic ability toward electrochemical proton reduction of sulfur-bridged trinuclear molybdenum complexes. **K. Kawamoto***, A. Ichimura, H. Hashimoto, I. Kinoshita, M. Hirotsu, T. Nishioka, Y. Hayashi
- 592.** Redox properties of linear octanuclear palladium complexes supported by tetraphosphine ligands. **K. Nakame**, B. Kure, T. Nakajima, T. Tanase*
- 593.** Molecular mechanisms for enhanced thermal and light stabilities of flavonoids by metal cations and polysaccharide. **T. Ohno***, N. Tachibana, A. Urabe, H. Otake, Y. Kimura
- 594.** Acid-induced vapochromism on a charge-transfer salt composed of an organic acceptor and an iron(II) complex. **R. Tanaka**, N. Matsushita*
- 595.** Synthesis of bis-cycles linked by aromatic rings and complexing property toward silver ions. **M. Iwase**, M. Ikeda, C. Kachi-Terajima, S. Kuwahara, Y. Habata*
- 596.** Humidity-dependence of luminescent property on a charge-transfer salt composed of tetracyanoplatinate(II) and an organic acceptor cation. **A. Kato**, W. Ueno-hara, N. Matsushita*
- 597.** Self-assembled construction of M₂L₄ cage complex for visual detection of ClO₄⁻. **A. Sonoya**, A. Handa, M. Kondo
- 598.** Controlling aperophilicity in an emissive dinuclear Au(I) building block towards co-ordination polymers for sensing toxic gases. **R.J. Roberts**, D. Le, D.B. Leznoff
- 599.** Incorporation of a halide anion guest into an inorganic bowl cavity. **S. Kuwajima**, Y. Kikukawa, Y. Hayashi*
- 600.** 3D coordination polymer for removal of perchlorate ion from aqueous solutions. **M. Sato**, E. Inoue, M. Kondo
- 601.** Molecular capsules that trap perchlorate ion and alkali cation. **R. Suzuki**, T. Inoue, K. Yananishi, M. Kondo
- 602.** Thermoresponsive 2D Ag(I) sheet as- sembly in the crystalline state using an assembled dipeptide ligand as a tem- plate. **R. Miyake**, Y. Nakagawa
- 603.** Harnessing weak interactions toward the synthesis of highly birefringent coordination polymers. **J.R. Thompson**, V.E. Williams, D.B. Leznoff*
- 604.** Mechanochemically induced structural transformation in [(3,6-dimethoxy-1,2,4,5-tetraene)silver(II)]X (X = CF₃SO₃, ClO₄) involving anion- π interactions. **J. Lee**, P. Kang, H. Kang, M. Choi*
- 605.** Linear hexanuclear platinum trihydride complex supported by triphosphine ligands. **K. Yamamoto**, K. Nakamae, B. Kure, T. Nakajima, T. Tanase*
- 606.** Cluster-to-cluster transformations: Controlled self-assembly of luminescent polynuclear gold(I) μ_3 -sulfido clusters. **L. Yao**, F. Hau, V. Yam
- 607.** Properties of a series of M₂M' type heterometallic trinuclear complexes containing N-heterocyclic carbene and triply bridging sulfide ligands. **Y. Maeda**, H. Hashimoto, T. Nishioka*
- 608.** Lattice dynamics of charge-separated ionic crystals of an Au₂Co³⁺₂ hexanuclear complex. **T. Kojima**, N. Yoshinari, M. Kawano, T. Konno*
- 609.** Development of a one-step selective hydroxylation of benzene with hydrogen peroxide catalyzed by Tris(2-pyridylmethyl)amine copper(II) complex. **M. Yamada***, K.D. Karlin, S. Fukuzumi
- 610.** S-bridged multinuclear palladium(II) complexes with aminothiolate-type li- gands. **M. Kouno***, Y. Miyashita, T. Konno
- 611.** Reactivity of D-penicillaminato cobal- t(III) complex toward copper(II). **N. Oya**, N. Yoshinari, A. Igashira-Kamiyama, T. Konno
- 612.** pH-Controlled chiral inversion and molecular dimerization in a gold(I)-cobalt(III) system with S-containing amino carboxy-lates. **S. Surin Wong***, P. Lee, A. Igashira-Kamiyama, T. Konno
- 613.** Vapochromic and mechanochromic be- havior of platinum(II) complexes with mixed polypryidine and thioglucose. **N. Kuwamura**, N. Kitani, T. Tsuge, T. Tsukuda, T. Konno
- 614.** Coordination behavior of a trigold(I) metalloligand with mixed tripododal triphos- phine and D-penicillaminato. **K. Imanishi***, Y. Hashimoto, N. Yoshinari, T. Konno
- 615.** Formation and interconversion of gold(I)-nickel(II) multinuclear complexes with mixed thiomalic acid and diphos- phines. **K. Igawa***, N. Yoshinari, T. Konno
- 616.** Coordination behavior of digold(I) met- alloligands with mixed diphosphine and D-penicillaminato toward nickel(II). **T. Itai**, A. Igashira-Kamiyama, N. Matsushita, T. Konno
- 617.** Parity-controlled formation of gold(I)-copper(II) supramolecular helices with penicillamine and bis(diphenylphosphino)-alkane. **N. Yoshinari***, A. Kakuya, T. Konno
- Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4
- Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170)**
- Organized by: K. Theopold, K. Mashima, Z. Xie
Presiding: K. Mashima
- 8:00 – 618.** Group 4 metal-catalyzed olefin oligomerization for natural product syn- thesis. **K. Nozaki**
- 8:30 – 619.** Addition reactions across metal-nitrogen multiple bonds in niobium bi- s(Imido) complexes. **B.M. Kriegel**, L. Grant, A. Obenhuber, R. Bergman, J. Arnold*
- 8:50 – 620.** Hydrohydratization of alkynes via C-H bond activation pathways and other element-hydrogen bond cleavage/nitrogen-element bond forming reactions of titanium hydrazido compounds. **P. Mountford***
- 9:20 – 621.** Synthesis and characterization of the homoleptic Group 5 ketimide com- plexes, M(N=C^tBu₂)₄ (M = V, Nb, Ta). P.L. Damon, J. Telser, **T. Hayton**
- 9:40 – 622.** Electronic vs. steric effects in the reactivity of aryloxo vanadium(III) and (IV) compounds with carbon dioxide. **C.J. Viasus**, N. Alderman, S. Gambarotta, I. Korobkov
- 10:00 – 623.** Carbon–carbon bond cleavage and rearrangement of benzene by a multinuclear titanium hydride complex. **S. Hu**, T. Shima, X. Kang, G. Luo, Y. Lu, Z. Hou*
- 10:20 – 624.** Molecular titanium nitrides: New synthetic entries and reactivity. **D. Mindiola**
- 10:50 – 625.** Direct evidence for [4+2] cy- cloaddition mechanism of alkynes to tan- tallacyclopentadiene as a model of alkyne cyclotrimerization. **K. Yamamoto***, H. Tsurugi, K. Mashima
- 11:10 – 626.** New group VI amide com- plexes and reactivity. **J.M. Smith**, R.K. Thomson*
- 11:30 – 627.** Addition to metal-metal δ bonds. **Y. Tsai**
- Hawaii Convention Center
Halls I, II, III
- Innovative Approaches in Bond-Cleavage and Bond-Forming Reactions at Late Transition-Metal Centres (#186)**
- Organized by: M. Hirano, D. Fogg, A. Veige
Presiding: D. Fogg, M. Hirano, A.S. Veige
- Poster Session**
10:00 – 12:00
- 628.** Synthesis, characterization, and unique catalytic activities of a fluorinated nickel enolate. **R. Doi**, M. Hashi, S. Ogoshi*
- 629.** Reversible transformation between phosphinite-Ni(0) and phosphide-Ni(II) via migratory alkoxide group transfer. **S. Kim**, Y. Kim, S. Oh, Y. Lee*
- 630.** Deep and ultra deep hydrodesulfurizations: Increased reactivity of a poly- nuclear nickel cluster toward difficult C–S bond activations. **M.M. Shoshani**, S.A. Johnson*
- 631.** Mechanistic study on C–C bond forma- tion of a nickel(II) monocarbonyl species with alkyl iodide. **C. Yoo**, J. Choi, Y. Lee*
- 632.** Synthesis and reactivity of PCS bis-pincer palladium and nickel complexes. **W. Shi***, L.P. Press, O.V. Ozorov
- 633.** Radical perspective on palladium: Li- gand-centered redox chemistry. **C.A. Sanz**, R. Hicks
- 634.** C-P palladacycles as catalysts for asymmetric synthesis of P-chiral diaryl- phosphinates. **J. Chiew**, P. Leung*
- 635.** Markovnikov-selective catalytic hy- drosilylation of electron-deficient alkenes by a mono(phosphine)palladium(0) com- plex. **R. Suda**, M. Abe, N. Komine, M. Hirano*
- 636.** Formation of indium-iron complexes and the catalytic activity toward double hydrosilylation of nitrile. **M. Ito**, M. Itazaki, S. Nakashima, H. Nakazawa*
- 637.** Synthesis and photophysical properties of rhodium complexes having fluorene- based diphosphine ligands. **Y. Matsusaka**, K. NOMURA, A. Inagaki
- 638.** C–H silylation reactions of arylalkynes catalyzed by 16-electron ruthenium com- plexes having a xanthene-based bis(silyl) ligand xanttil. **T. Kitano**, T. Komuro, H. Tobita*

*** Principle Author**

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<http://pacificchem.org/onlineprogram>

- 639.** Ruthenium-catalyzed monoalkenylation of aromatic ketones via selective aromatic carbon–heteroatom bonds cleavage. **H. Kondo**, N. Akiba, T. Kochi, F. Kakuchi*
- 640.** 2:1 Coupling of terminal alkynes with secondary amines catalyzed by quinolinolato rhodium complexes. **M. Hamada**, K. Mochizuki, T. Kochi, F. Kakuchi
- 641.** Internal concerted carbocation transfer in formation of rutenacycle by C–O bond cleavage. **N. Araki**, T. Yasumuro, N. Komine, M. Hirano
- 642.** Remote rearrangement of the metal center in (η^6 -C₆Me₆)M(II) (M = Ru, Os) complexes. **K. Takano**, Y. Ikeda, S. Kodama, Y. Ishii*
- 643.** Syntheses and reactivities of phosphine–quinolinolato rhodium complexes: Formation of vinylidene-bridged dirhodium complexes. **S. Takano**, T. Kochi, F. Kakuchi*
- 644.** Synergy effect between lithium hydride and iron used in ammonia synthesis. **W. Peikun**, J. Guo, F. Chang, P. Yu, W. Gao, G. Wu, P. Chen
- 645.** Evaluation of a silane–cobalt interaction in the synthesis of a silyl cobalt(II) complex. **J. Kim**, K. Park, S. Kim, Y. Lee*
- 646.** Hindrance to cyclometalation: A study on N-demethylation triggered from ortho-metallation of sterically-hindered ligands. **H.J. Chen**, R.H. Teo, J. Wong, Y. Li, S.A. Pullarkat, P. Leung*
- 647.** Reactivity study of nickel amido complexes supported by a diphosphinosilyl ligand. **K. Park**, J. Kim, Y. Lee*
- 648.** Efficient iron and aluminum catalysts for coupling reaction of CO₂ and epoxides. **C. Bae**, J. Kim, Y. Lee*
- 649.** Mixed ligand approach to palladium-catalyzed direct arylation polymerization (DAPr): Synthesis of DA polymers with diketopyrrolyrrole units. **R. Takahashi**, E. Mizuki, M. Wakioka, F. Ozawa*
- 650.** Base metal catalysts for petroleum and biomass hydrotreatment. **O. Brown**, J.M. Stryker*
- 651.** Synthesis of pincer-type nickel(II) complexes and application to nickel-catalyzed cross-coupling reaction of aryl halides with arylmagnesium halides. **Y. Yamaguchi***, E. Asano, N. Kurisu
- 652.** Palladium and nickel NNN-pincer complexes and their ability to stabilize oxygen containing moieties. **M. Lim***, R. Roesler, Y. Jiang
- 653.** Inductive effects of substituted pyridyl-indole ligands on Pt catalyzed hydroarylation. **B.A. Suslick**, A.L. Liberman-Martin, T. Tilley*
- 654.** Mixed ligand approach to palladium-catalyzed direct arylation polymerization (DAPr): Synthesis of DA polymers with dithienosilole units. **E. Iizuka**
- 655.** Oxidative addition of oxime derivatives to transition metal complexes followed by C–H activation: Mechanistic consideration and synthetic application. **T. Shimbayashi**, K. Okamoto*, K. Ohe*
- 656.** Selective alkene insertion into transition metal–hydrogen bonds assisted by mono(phosphorus ligand)palladium(0) complexes. **N. Komine***, R. Ito, H. Suda, M. Hirano, S. Komiya
- 657.** Structures and chemical reactivity of binuclear Pd and Ru complexes with N,S,S,N-ligands containing the *ortho*-aminophenol motif. **M. Bierenstiel***
- 658.** Control of reaction selectivity in palladium-catalyzed transformations through fine tuning of ligand structures. **K.H. Shaughnessy***
- 659.** R/X exchange reaction on Pd and Pt complexes with phosphine ligand, *cis*–[MR₂(P(NMeCH₂)₂X)₂] (M = Pd, Pt) via an intermediate of phosphonium complex. **M. Itazaki***, Y. Shigesato, N. TSUCHIDA, K. Takano, H. Nakazawa*
- 660.** Unusual α -selective hydrosilylation of electron-deficient alkynes using rhodium(I) dithiolate complex. **T. Sato***, H. Yashiki, H. Takano, D. Kanno, S. Oi
- 661.** Efficient dehydrogenation of formic acid using bifunctional iridium complexes bearing sulfonyldiamine ligands. **A. Matsunami***, Y. Kayaki, T. Ikariya

- 662.** [3,3]-Sigmatropic rearrangement of pyridyl ketone oxime esters at an Ir complex. **H. Takahashi**, S. Kodama, Y. Ishii*
- 663.** Synthesis of amine and imine from thioamide through the desulfurization by hydrosilane with the help of an iron complex. **K. Fukumoto**, A. Sakai, H. Nakazawa*
- 664.** Catalytic cross-dimerization of diarylacetylene with methyl methacrylate by a ruthenium(0) complex. **S. Kiyoata**, S. Watanabe, N. Komine, S. Komiya, M. Hirano*
- 665.** Three component coupling reaction of alkene, alcohol, and sodium formate through chelation assisted O–H bond cleavage by Ru(0) complex. **W. Park**, C. Lee, D. Kim, C. Jun*
- 666.** Ru₃(CO)₁₂-catalyzed chemical modification of polybutadiene with ester functionality through chelation-assisted O–H bond cleavage of alcohol. **C. Lee**, W. Park, D. Kim, C. Jun*
- Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2
- Transition Metal Complexes of N-Heterocyclic and Mesocyclic Carbenes: Structure, Materials and Catalytic Applications. (#195)**
- Organized by:* C. Crudden, S. Chang, M. Albrecht, D. Allen, U. Complete
- 8:00 – 667.** Protic N-heterocyclic carbenes – synthesis and reactivity. **E. Hahn***
- 8:30 – 668.** Singlet carbenes for the isolation of highly reactive transition metal complexes. **G. Bertrand**
- 9:00 – 669.** Carbon–element bond forming reactions with f-block NHC complexes. **P.L. Arnold**, N. Bell, T. Cadenbach, K. Wang, I. Marr, Z. Turner, R. Tooze, M. McMullen, J. Rieb, F. Kuhn, A. Fyfe
- 9:30 – 670.** Controlled assembly of NHC self assembled monolayers on gold. **C.A. Smith**, M. Narouz, C. Crudden*
- 9:50 – 671.** Carbodicarbene complexes of ruthenium: highly active catalysts for the hydrogenation of olefins. **C. Pranckevicius**, D. Stephan*
- 10:10 – 672.** Rollover cyclometalation pathway in rhodium catalysis: Dramatic NHC effects in the C–H bond functionalization. **S. Chang**
- 10:30 – 673.** N-heterocyclic carbene as a ligand and a catalyst for atom-economical and selective C–N and C–C bond formation reactions. **S. Hong***
- 11:00 – 674.** Catalytic synthesis of benzoxasiloles via activation of organosilanes using γ -aldehyde nickel(0)/N-heterocyclic carbene complex. **Y. Hoshimoto***, R. Kumar, M. Ohashi, S. Ogoshi
- 11:20 – 675.** Exploring the geometric and electronic structure of oxidatively activated iridium carbene water oxidation catalysts. **P. Kenneppohl***
- 11:40 – 676.** NHC ligation for metal-chalcogenide cluster assembly. **J.F. Corrigan**, M. Azizpoor Fard
- Hawaii Convention Center
Halls I, II, III
- Nuclear Probes in Nanoscale Characterization (#254)**
- Organized by:* M. Takahashi, A. Hill, V. Sharma, J. Wang, M. Takahashi, M. Takahashi, K. Nomura, Y. Yamada
- Poster Session**
10:00 – 12:00
- 677.** Monitoring of the changes of iron forms in Fe/AC catalysts during catalytic wet peroxide oxidation of m-cresol using Mössbauer spectroscopy. **Y. Wang**, H. Wei, P. Liu, J. Wang, X. Li, Y. Zhao, C. Sun*

- Hawaii Convention Center
Halls I, II, III
- Metal-containing ?-Conjugated Systems: Syntheses, Properties, Applications (#269)**
- Organized by:* M. Humphrey, V. Yam, M. Akita
Presiding: M. Akita, M. Humphrey, V. Yam
- Poster Session**
10:00 – 12:00
- 678.** Donor–Acceptor–Donor nature of nickel bimetal dithiine complex bridged by tetraethoxalate (tto) skeleton and its potential use for a closed shell single component molecular conductor. **M. Hayashi***, K. Otsubo, M. Maesato, K. Sugimoto, A. Fujiwara, H. Kitagawa
- 679.** Ferrocene- and cyclopentadiene-fused acenes and tropones. **B. Maherjan**, **J.P. Selegue***, S. Parkin
- 680.** Synthesis and characterization of group 10 metal complexes with indigo-like ligands. **D.T. Hofsommer**, R. Hicks*
- 681.** Toward the synthesis of new dyes, ligands, and complexes inspired by dipyrromethenes. **G.N. Boice**, R. Hicks
- 682.** Multistory discrete Pd(II) complexes: Construction, molecular behavior, and properties. **H. Lee**, O. Jung
- 683.** Visible-light driven homo- and copolymerization of styrenes by bichromophoric Ir-Pd photocatalyst. **A. Inagaki***, K. Saito, S. Kikuchi, K. Murata, M. Akita
- 684.** Theoretical study on the open-shell characters and third-order nonlinear optical properties of organometallic compounds. **S. TAKAMUKU**, Y. Kitagawa, M. NAKANO
- 685.** Metal complexes of a quadruply fused porphyrin: Structure, redox properties, and Lewis acidity of the central metal ion. **T. Ishizuka***, K. Komamura, Y. Saegusa, T. Kojima
- 686.** Diverse copper(I) ethylene complexes with related 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine ligands. **M. Maekawa***, T. Okubo, T. Kuroda-Sowa, M. Munakata
- 687.** Synthesis of multinuclear Ru–Fe metal–ladiitholene complexes. **T. Sagawa***, S. Tsukada, T. Gunji
- 688.** Dinuclear complexes with a fused ligand having phthalocyanine and Schiff-base coordination sites. M. Handa, **K. Wada**, K. Murakoshi, Y. Kataoka, M. Mikuriya
- 689.** Dinuclear complexes with a fused ligand having phthalocyanine and salen-like coordination sites. **M. Handa**, K. Kanagawa, K. Fujii, T. Ikeue, Y. Kataoka, T. Sugimori, M. Mikuriya
- 690.** Anomalous thermal behaviour of [Ni(salen)] derivatives having methyl substituent groups at nitrogen bridge. **T. Yoshida***, K. Taniguchi, S. Ichimura, Y. Tamaki, K. Miyamura
- 691.** Synthesis of cobalt dithioline complex having dihalobenzenediimidolate ligand. **M. Kondo**, S. Tsukada, T. Gunji*
- 692.** Evaluation of electronic communication of dinuclear mixed-valence complexes by the IR spectroscopic method. **H. Takahashi**, Y. Tanaka, M. Akita*
- 693.** Synthesizes and properties of molybdenum dithioline complexes. **N. Abe**, S. Tsukada, T. Gunji*
- 694.** Research about the structure of Ba₂[Ni(pdtt)₂]₁·1H₂O (pdtt = 2,3-pyrazinediimidolate) and its magnetic and electric properties. **M. Kanari**, H. Iguchi, S. Takaishi, B.K. Breedlove, K. Kagesawa*, M. Yamashita*
- 695.** Thermal behavior of Ni, Cu, and Pd complexes of phenylalkylene substituted salicylaldimine. **Y. Shioya***, M. Saeki, A. Honda, Y. Tamaki, K. Miyamura
- 696.** Synthesis of insulated molecular wires functionalized by metals coordination to their backbones. **T. Hosomi**, H. Masai, J. Terao, T. Fujihara, Y. Tsuji
- 697.** Enhanced phosphorescence in the solid state by cyclic insulation of platinum-acetylidyne polymers. **H. Masai**, J. Terao, S. Makuta, Y. Tachibana, T. Fujihara, Y. Tsuji

- 698.** Mono- and dinuclear Ru(dppz) DNA light-switch complexes incorporating groove-binding tethers. **H. Saeed**, J. Thomas*
- 699.** Pentptycene-incorporated tridentate platinum(II) alkynyl complexes: Synthesis, photophysical properties, and mechanochromicity. **C. Lin***, J. Yang
- 700.** Ruthenium alkynyl-functionalized tris-(phenylpyridine)iridium complexes. **M. Cifuentes***, H. Zhao, P. Simpson, M. Morshed, A. Barlow, G. Mohey, M. Humphrey*
- 701.** Synthesis and photophysical characterization of some binuclear gold(I) alkynyls with phenanthryl-based bridges. **B. Babgi***, M. Humphrey
- 702.** CAC vs. ACC (A = S, Se, Te, BOMe, Sm₂Pr₂; R = Cl, Ph, Cy) bridged bimetallics. **R.A. Manzano**, A.L. Colebatch, **Y. Han**, A.F. Hill*, K.M. von Nessi, R. Shang, M. Sharma, J.S. Ward
- 703.** Selenium-interrupted carbonchain bridged bimetallics. **R.A. Manzano**, T. Evers, A.F. Hill*, J.S. Ward
- Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1
- Metal Mediated Polymerization (#292)**
- Organized by:* P. Hayes, R. Waterman, T. Mizuta, Y. Tang, P. Sangstrutnugul
Presiding: P.G. Hayes, J. Okuda
- 8:00 Introductory Remarks**
- 8:05 – 704.** Control of metal-mediated olefin polymerizations through the first and second ligand sphere. **J. Okuda***
- 8:35 – 705.** Cooperative effects in homo- and heterobimetallic catalysts for ethylene polymerization/copolymerization. **M. Delferro**, T.J. Marks
- 8:55 – 706.** Synthesis of (Imido)niobium(V) complexes as catalyst precursors for olefin polymerization. **N. Srisupap**, K. NOMURA*
- 9:15 – 707.** Structures of α -, β - and γ -agostic species alkyltitanocene complexes. **M.C. Baird***, A. Dunlop-Brière, P.H. Budzelaar
- 9:45 Intermission**
- 10:00 – 708.** Precise synthesis of fine polyolefins by ethylene copolymerization with sterically encumbered monomers, cyclic olefins, and with comonomers containing reactive functionality. **K. NOMURA***
- 10:30 – 709.** Using the coordination chemistry toolbox for polymerization catalysis. **C. Redshaw***
- 10:50 – 710.** Iron-catalyzed homo- and copolymerization of propylene. **T. Kawakami**, S. Ito, K. Nozaki*
- 11:10 – 711.** New insight into the early stages of reaction by the self-initiating Phillips ethylene polymerization catalyst. **S.L. Scott***, Y. Wang, A. Fong, B. Peters
- Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2
- Novel Heme Proteins and Model Systems (#305)**
- Organized by:* J. Dawson, T. Hayashi, M. Stillman
Presiding: M. Stillman
- 8:00 break**
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- * Principle Author
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- 8:40 – 712.** Using heme to make a heme: The unusual chemistry and biology of HemQ. **J. DuBois**, A.I. Celis, G.S. Lukat-Rodgers, K. Rodgers
- 9:00 – 713.** Interplay of structure, dynamics, and protein-protein interactions enable bacterioferritin's central role in bacterial iron homeostasis. **M. Rivera***, H. Yao, S. Lovell, Y. Wang
- 9:20 – 714.** Heme uptake in pathogenic bacteria: *Streptococcus pyogenes* and *Corynebacterium diphtheriae*. **D.W. Dixon***
- 9:40 – 715.** Elucidating the biosynthesis and transport of heme A. **E.L. Hegg**, E. Herwaldt, E. Rivett, A. White
- 10:00 – 716.** Heme transport and metabolism in *Yersinia pseudotuberculosis*. **S. Ozaki***, S. Nagano, T. Hino
- 10:20 – 717.** H₂O₂-dependent hydroxylation of C-H bond by myoglobin reconstituted with a manganese porphyrin complex. **K. Oohora***, T. Hayashi
- 10:40 – 718.** Investigating the mechanism of signal transduction within globin coupled sensors. **E.E. Weinert***, J.L. Burns
- 11:00 – 719.** Fine-tuning heme protein model myoglobin by post-translational modification. **Y. Lin***
- 11:20 – 720.** Effect of polar functional group at the distal side of the myoglobin model complex on its ligand binding property (O₂ and CO) in aqueous solution. **H. Kitagishi***, N. Kitamura, K. Kano
- 11:40 – 721.** Electronic control of myoglobin function. **Y. YAMAMOTO***, R. NISHIMURA, Y. KANAI, T. SHIBATA, S. YANAGISAWA, T. OGURA, H. TAI, T. Matsuo, S. Hirota, S. Neya, A. SUZUKI
- Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2
- Metal Coordination Sphere Design for Challenging Bond Transformations (#318)**
- Organized by: K. Caulton, A. Hill, S. Johnson, M. Yamashita
Presiding: K. Caulton, C. Lu
- 8:00 Welcome Remarks**
- 8:05 – 722.** Hydroarylation of olefins using Ru(II) catalysts: Influence of ancillary ligand. **T.B. Gunnو***, S.A. Burgess, E.E. Joslin, T.R. Sundari, M. Sabat, W.H. Myers
- 8:25 – 723.** Transfer, metathesis, and cationation: Reactivity patterns emerging from borylene complexes. **H. Braunschweig**
- 8:45 – 724.** Hemilabile N,O-chelating ligands: Dynamic coordination modes for promoting reactivity and hydroaminoalkylation catalysis. **L.L. Schaefer***
- 9:05 – 725.** Iron-catalyzed cross-coupling aided by olefin substituents. **A. Jacobi von Wangenheim**
- 9:20 – 726.** Donor properties and high valent metals: Parameterizing catalyst rates and other properties. B. Billow, T. McDaniel, A. Odom*
- 9:35 – 727.** Synthesis, design, and catalytic applications of trianionic pincer ligands in transition metal chemistry. **A.S. Veige**, S.S. Nadif, M.E. O'Reilly, S. VenkatRaman, I. Ghiviriga, K.A. Abboud
- 9:50 – 728.** Metalatorless aerobic C–H oxidation by a Pt(II)/Pt(IV) redox couple. **D.B. Watts**
- 10:05 – 729.** Making C–H bonds with CO₂: Tuning molecular iron electrocatalysts with ligand design. A. Taheri, N.D. Loewen, **L.A. Berben***
- 10:25 – 730.** Antimony Lewis acids in the secondary coordination sphere of gold complexes: An opportunity for redox-controlled catalysis. H. Yang, **F.P. Gabbaï**
- 10:45 – 731.** Modifications to the geometry and reactivity of low-coordinate Fe(II) complexes through modular ligand design. **N.M. Hein***, T. Suzuki, T. Ogawa, M. Fryzuk
- 11:00 – 732.** Oxidative addition of chlorohydrocarbons to a rhodiumtrispyrazolylborate complex. **W.D. Jones***, Y. Jiao
- 11:15 – 733.** Facile synthesis and versatile reactivity of cyclometalated Rh⁴⁺ and Ni^{II} pincer complexes. **J. van der Vlugt***

- 11:30 – 734.** Investigating the flexibility of the catalytic pocket in transition metal complexes. **L. Cavallo***, L. Falivene, R. Credendino
- 11:45 Flash Presentation 1**
- Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2
- Dioxo Activation Chemistry of Metalloenzymes and Models (#339)**
- Organized by: A. Rosenzweig, S. Itoh, W. Nam
Presiding: W. Nam
- 8:00 – 735.** Oxygen activation at diiron cluster-containing oxygenases: Structures of key intermediates. R. Banerjee, C.J. Knot, A. Komor, B.S. Rivard, A.J. Jasinski, L. Que, **J.D. Lipscomb***
- 8:30 – 736.** Demystifying the chemical magic of non-heme-iron enzymes in natural product biosynthesis. **J.M. Bollinger**, C. Krebs
- 9:00 – 737.** Mechanisms of enzymatic thiol dioxygenation. **G.N. Jameson***
- 9:30 – 738.** Amazing high-valent iron-oxo reaction landscape. **L. Que***
- 10:00 – 739.** Carbonylamido ligand effect on the nature of mononuclear nonheme oxiron species. **Y. Hitomi**
- 10:30 – 740.** Dioxygen activation and oxygen-functionalization of C–H and C=C bonds by biomimetic iron complexes. **T.K. Paine***
- 11:00 – 741.** Chemistry without cofactors: How an extraordinary family of enzymes activates O₂. **J. DuBois**, M. Machovina, V. Smirnov
- 11:30 – 742.** Biomimetic metal–oxygen intermediates in dioxygen activation chemistry. **W. Nam***
- Hawaii Convention Center
Halls I, II, III
- New Frontiers in Bioinorganic Chemistry (#356)**
- Organized by: M. Yamaguchi, S. Cohen, X. Ottenwaelder
- Poster Session**
10:00 – 12:00
- 743.** Effect of chemical structure of artificial co-enzyme with 4,4'-bipyridine skeletons on the CO₂ reduction catalytic activity with formate dehydrogenase. **S. Ikeyama**, Y. Amao
- 744.** Roles of N- and C-terminal domains in the ligand binding properties of cytoglobin. **S. Hanai**, H. TSUJINO, R. YANASAKA, T. YAMASHITA, T. UNO
- 745.** Dinuclear nickel complex modeling the functions of nickel superoxide dismutase. **T. Shimodaira***, Y. Kataoka, T. Kawamoto
- 746.** Syntheses of far-red-absorbing porphyrin derivatives and photodynamic antimicrobial activities. **y. iwasaki**, R. Higashino, M. Nakai, R. Clarke, T. Storr, S. Yano, Y. Nakabayashi
- 747.** Metal complexes of the antiparasitic drug Metronidazole. J.H. Palmer, J. Wu, **R.K. Upmacis***
- 748.** Biophysical analysis of anticancer platinum complex binding to DNA and proteins – a multifaceted approach. **B.J. Pages**, J. Sakoff, J. Gilbert, A. Rodger, N. Jones, D.L. Ang, J. Aldrich-Wright*
- 749.** Anticancer effects of a new aminoguanconjugated platinum complex anticancer agent against gastric cancer cells. **S. Yano***, N. Hayashi, H. Kataoka, K. Kawamoto, T. Shibahara, Y. Kinosita, A. Nomoto, A. Ogawa, K. Morimoto
- 750.** Cancer and cell resistance: Optimised methods for the preparation of platinum and ruthenium complexes as selective chemotherapeutic agents. **R.I. Taleb***, N. Mansour, S. Mehnana, B. Bassil, C. Daher, M. Mroueh, M. El-Sibai
- 751.** Control of photochemical ligand exchange reaction of ruthenium complexes by addition of acid or base. **A. Kobayashi**, M. Yamaguchi, K. Sato
- 752.** Investigating the biological activity and therapeutic potential of ruthenium (II) tpm compounds. **A. Militan***, M.R. Gill, **R.L. Mowll**, J. Thomas, C. Smythe
- 753.** Simple alternatives to TPP as enhanced mitochondrial delivery agents. **f. garcia***, Z. Hu, E.K. Yeow
- 754.** Development of multifunctional small molecules that modulate metal–Aβ interactions toward treating Alzheimer's disease. **M. Jones***, E. Matheiu, T. Storr
- 755.** Effect of 5-aminolevulinic acid on cytochrome P450-based prodrug activation. **M. Miura***, K. Ito, M. Hayashi, T. Tanaka, I. Okura, S. Ogura
- 756.** Syntheses of Re and ^{99m}Tc CAIX inhibitors for cancer diagnostics. **M. Nakai***, J. Pan, K. Lin, J.R. Thompson, Y. Nakabayashi, T. Storr
- 757.** Cointercalation of doxorubicin and cis-platin anticancer drugs into zirconium phosphates nanoparticles for drug delivery applications. **J.R. Gonzalez-Villegas***, J. Colon
- 758.** Artificial biocatalysts with a covalently-linked copper terpyridine complex embedded within the cavity of nitrobindin. **T. Hinimaya**, D. Sauer, A. Onoda, J. Okuda, T. Hayashi
- 759.** Advanced EPR characterization of the copper-amyloid peptides. **S. Kim**
- 760.** Reaction dynamics for the C–H bond activation by iron(IV)-oxo complexes: Natural vs. biomimetic systems. **B.K. Mai**, Y. Kim*
- 761.** CO₂ and CO transformation at a nickel center supported by a pincer-type PNP ligand. **C. Yoo**, Y. Lee*
- 762.** Carbon dioxide activation inspired by the CODH active site. **Y. Kim**, J. Kim, Y. Lee*
- 763.** Nickel, palladium, and platinum complexes with multidentate sugar incorporated N-heterocyclic carbene ligands. **T. Nishioka***, Y. Maeda, Y. Imanaka, H. Hashimoto
- 764.** Ferrocenyl histidine conjugates and its interactions with zinc, cadmium and other metal ions. **A. Ferranca***, H. Kraatz
- Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3
- Isotope Production--Providing Important Materials for Research and Applications (#363)**
- Organized by: D. Phillips, K. Gagnon, Y. Hatsukawa
Presiding: Y. Hatsukawa, A. Shinohara
- 8:00 – 765.** Recovery of enriched Mo targets for economic production of ^{99m}Mo medical isotope without use of highly enriched uranium. **P. Tkac**, G.F. Vandegrift
- 8:20 – 766.** Preparation of ^{99m}Tc and ¹²⁴I for use of nuclear medicine. **N. Takahashi***, Y. Hayashi, K. Nakai, A. Shinohara, H. Ikeda, J. Hatazawa, M. Fukuda, K. Hatano
- 8:40 – 767.** Medical radioisotope production with accelerator neutrons by deuterons. **K. Tsukada***, N. Sato, S. Watanabe, N.S. Ishioka, Y. Hatsukawa, K. Hashimoto, T. Kin, S. Takeda, M. Kawabata, H. Saeki, Y. Nagai
- 9:00 – 768.** High power solid target station and turnkey system for the production of ^{99m}Tc on the GE PETtrace cyclotron. **M.S. Kovacs***, N. Cockburn, J. Corsaut, K. Buckley, V. Hanemayer, J. Klug, S. Zeisler, J. Tanguay, A. Cellier, F. Prato, J. Valliant, T. Ruth, F. Benard, P. Schaffer
- 9:20 – 769.** Production of medical radioisotopes including ⁹⁹Mo by using accelerator neutrons. **Y. Nagai***, M. Kawabata, K. Hashimoto, Y. Hatsukawa, H. Saeki, S. motoishi, K. Tsukada, A. Ohta, T. Shina, Y. Kawauchi
- 9:45 Break**
- 10:00 – 770.** Cyclotron produced ^{99m}Tc: Downstream processing optimization and automation. **J.D. Andersson***, J.S. Wilson, B.A. Thomas, A.J. McEwan, D.N. Abrams, S.A. McQuarrie, K.M. Gagnon
- 10:20 – 771.** Experimental validation for optimization of transcurium isotope production: Target design, fabrication, and processing. **J. Burns***, S. Hogle, C. Alexander, J. Ezold
- 10:40 – 772.** Neutron flux filtering for the optimization of transcurium isotope production. **S. Hogle***, C. Alexander, J. Burns, J. Ezold
- 11:00 – 773.** Production of ^{95m}Tc for Compton Camera imaging. **Y. Hatsukawa***, K. Tsukada, K. Hashimoto, T.K. Sato, M. Asai, A. Toyoshima, Y. Nagai, T. Tanimori, S. Sonoda, s. kabuki, H. Kimura
- 11:20 – 774.** Measurement of production cross sections of Tc and Re isotopes in deuteron-induced reactions on ^{nat}Mo and ^{nat}W up to 24 MeV. **M. Komori***, M. Murakami, H. Habu
- 11:40 – 775.** Production of exotic radionuclides at the PSI Accelerator Complex. **E.A. Mauger***, R. Dressler, S. Heinitz, M. Schumann
- Hilton Hawaiian Village
Rainbow Tower, Rainbow 2
- Telomeres and other G-quadruplex Structures as Targets for Metallodrugs (#459)**
- Organized by: J. Aldrich-Wright, N. Sugimoto, J. Chaires, S. Ralph
Presiding: J. Aldrich-Wright, S.F. Ralph
- 8:00 Welcome**
- 8:00 – 776.** Understanding the roles of the G-quadruplex and i-motif alongside supercoiling in the MYC promoter as a basis for the development of new therapeutic strategies. **L.H. Hurley***, C. Sutherland, V. Gokhale
- 8:30 – 777.** Selective recognition of thymine containing loops in G-quadruplexes by bifunctional Zn(II) complexes. **J.R. Morrow***, K. Sitters, M. Fountain
- 9:00 – 778.** Structural and mechanistic insights into catalytic heme-DNA/RNA complexes: From biology to green chemistry. **D. Sen***, N. Shumayirkh, T. Canale
- 9:30 – 779.** Ferrocenylnaphthalene diimide derivatives as a novel tetraplex DNA ligand. **S. Takenaka***
- 10:00 Morning tea break**
- 10:10 – 780.** C-quadruplex? Adventures with the "other" strand. E.P. Wright, Q. Sheng, H. Day, C.J. Morris, **Z.A. Waller***
- 10:40 – 781.** Determination of ligand-binding quartets in telomeric G-quadruplex by mechanochemical dissection. **C. Ghimire**, S. Park, C. Xu, H. Sugiyama, H. Mao*
- 11:00 – 782.** Optical probes for specific quadruplex DNA structures. **J. Thomas***
- 11:30 – 783.** G-quadruplexes regulate transcription and translation. **H. Tateishi-Karimata**, T. Endoh, S. Takahashi, **N. Sugimoto**

* Principle Author

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Thursday AfternoonHilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3**Functional Nanomaterials Based on Coordination Chemistry (#73)***Organized by:* T. Uemura,
M. MacLachlan, H. Matsui
Presiding: M. MacLachlan**13:00 – 784.** Shape-shifting supramolecular structures regulated through coordination chemistry. **C.A. Mirkin*****13:25 – 785.** Chemical and electrochemical switching of a ferrocene-based molecular rotor: Toward non-interlocked molecular actuators. **J.D. Crowley***, S.O. Scottwell, A.B. Elliott, K.C. Gordon, J. McAdam, K.J. Shaffer, A. Nafady**13:40 – 786.** Electrochromism in metallo-supramolecular polymers. **M. Higuchi*****14:00 – 787.** Coordination-based molecular assemblies as electrochromic materials: Ultrahigh switching stability and coloration efficiencies. **M. Lahav****14:15 – 788.** High-resolution separation of thiolate-protected gold clusters. **Y. Negishi*****14:35 Break****14:45 – 789.** Self-assembly approaches toward photon-harvesting and upconverting molecular systems. **N. Kimizuka****15:10 – 790.** Multifunctional nanoballs. **S.R. Batten****15:25 – 791.** Surface assisted self-assembly of porphyrin wires. **J. WEISS***, J.A. WYTKO, Y. KIKKAWA**15:45 – 792.** Control of the molecular orientation of metallocporphyrin on surface. **S. Yoshimoto*****16:05 – 793.** Investigating the role of defects in semiconducting polymer nanowires. **C. Luscombe*****16:25 – 794.** Selective synthesis of Co_8S_{15} cluster inside the bowl-shaped templating fullerene ligand. **Y. Matsuo***Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1**Coordination and Supramolecular Chemistry for Aqueous Metal Ion Separations (#97)***Organized by:* R. Ellis, D. Robinson, R. Motokawa**13:00 – 795.** Speciation of rare-earth-elements ions at liquid-vapor interfaces. M.K. Bera, G. Luo, M.L. Schlossman, L. Soderholm, S. Lee, **M.R. Antonio*****13:25 – 796.** Understanding of self-assembly of heteropolyanions in bulk aqueous solutions and at air-water interfaces. **M.K. Bera, M.R. Antonio****13:50 – 797.** Active interface in liquid/liquid extraction processes probed by non-linear optics and neutron/x-ray reflectivity: static and dynamics. **O. Diat***, E. Scoppola, H. El Ouazzani, J. Dufreche, D. Meyer, P. Guilbaud, A. Jonchere, P. Brevet, G. Fragneto, O. Konovalov, P. Gassian**14:15 – 798.** Understanding the structures of solvent extraction in the organic phase at the all-atmosphere resolution. **B. Qiao, M. Olvera de la Cruz, R. Ellis****14:40 – 799.** Cluster-based uranium separation chemistry with excellent atom economy. **M. Nyman**, H. Neal**15:05 Break****15:20 – 800.** Biomolecules for supramolecular separations of the actinides. **M. Jensen***, J. Gogolski**15:45 – 801.** Colloidal model for separation chemistry. **J. Dufreche**, T. Zemb, M. Duvail, A. Karmakar, Y. Chen, N. Nguyen, P. Guilbaud**16:10 – 802.** X-ray observations of ion-extractant complexes arrested at the oil-water interface during solvent extraction. **M.L. Schlossman*****16:35 – 803.** SANS and EXAFS study of hierarchical structure assembled by coordination species in biphasic solvent extraction. **R. Motokawa**, T. Kobayashi, H. Endo, S. Suzuki, T. YaitaHilton Hawaiian Village
Mid-Pacific Center, Coral 1**Frontiers of Molecular Magnetism (#109)***Organized by:* H. Oshio, J. Miller, R. Oakley, S. Brooker, S. Gao, M. Ohba
Presiding: R. Clerac, S. GAO**13:00 – 804.** Molecular magnetism controlled by solid-state electrochemistry. **K. Awaga*****13:30 – 805.** Weak ferromagnetic ordering of $\text{Li}[\text{TCNE}]$ (TCNE = tetracyanoethylene). **J.S. Miller**, J. Her, P. Stephens, R. Davidson, J. Novoa, F. Mota, F. Palacio**13:50 – 806.** Explaining the puzzling magnetism of two-coordinate first row transition metal complexes. L.M. Davis, C.F. Lovitt, C.M. Spicer, G.R. Potratz, B.B. Trinh, M.J. Nilges, S.A. Stoian, W.M. Reiff, G.S. Girolami**14:10 – 807.** Transport properties of pi-stacked radical polymer based on trioxo-triangulene neutral radicals. **Y. Morita***, C. Yamada, T. Torii, T. Murata**14:30 Break****14:45 – 808.** Lanthanide phosphonates with tunable magnetic behaviors. **L. Zheng****15:05 – 809.** Organometallic single-ion magnets. **S. GAO****15:25 – 810.** Self-assembly of coordination complexes with regular arraysof metal ions: Rings, helices, and grids. **T. Shiga***, H. Sato, G.N. Newton, H. Oshio***15:45 – 811.** Electronic, electrochemical, and magnetic properties of mixed-valence polyoxometalates with $3d^n/3d^{n-1}$ and $4d^1/4d^{n-1}$ configurations.**D. Venegas-Yazigi**, F. Fernandez-Vidal, J. Gonzalez, N. Soto, K. Wrighton, C. Aliaja, V. Paredes-Garcia, E. Spodine**16:05 – 812.** Protecting molecular spin qubits against dipolar decoherence. **S. Hill***, M. Shiddiq, D. Komijani, Y. Duan, S. Cardona-Serra, A. Gaita-Ariño, E. CoronadoHilton Hawaiian Village
Mid-Pacific Center, Nautilus 2**Electron Transfer and Electrochemistry of Inorganic and Organometallic Materials (#126)***Organized by:* H. Nishihara, P. Harvey, W. Wong
Presiding: T. Michinobu, H. Nishihara**13:00 – 813.** Photofunctional bottom-up bis-(dipyrrinato)zinc(II) complex nanosheet. **R. Sakamoto*****13:30 – 814.** Photofunctional 1D coordination polymer featuring bis(dipyrrinato)zinc(II) complex motif. **R. Matsukawa**, R. Sakamoto, H. Nishihara***13:50 – 815.** New redox-active multilayer thin films and their silver complexes by alkyne-acceptor click chemistry. **T. Michinobu*****14:40 – 816.** Controlling the charge state in heterolayer films of sequential assembled Ru complexes toward molecular memory devices. **M. Haga***, T. Nagashima, H. Ozawa**14:40 – 817.** External stimuli-induced intramolecular electron transfers in cyanide-bridged multinuclear complexes. **M. Nihei***, Y. Sekine, K. Shirayangai, H. Oshio**15:30 – 818.** Multi-electron redox tuning of bimetallic complexes with open coordination sites. **D. Villagrán***, K. Ventura, N. Valdez, Y. Wu, J. Veleta, A. Metta-Magana**15:30 – 819.** Valence-detrappling in the mixed-valence state of biosmocenium(II, IV) salts. H. Yasuhara, **S. Nakashima*****15:50 – 820.** $\text{Cu}(\text{II})/\text{Cu}(\text{II})$ electron transfer coupled to dioxygen activation in biomimetic complexes: Mononuclear vs. di-nuclear approach. **Y. LE MEST***, N. Le Poult, B. Douziech**16:20 – 821.** Electrochemical evaluation of pseudo-Jahn-Teller effects in polyoxometalate anions. **K. Eda***, K. Koike, H. Hirabaru, T. Ueda, T. Osakai**16:40 – 822.** Mechanism of the oxidation of acetylferrocene and 1-ferrocenylethanol by dicyanobis(phenaanthroline)iron(III). **R. Khattak***, I.I. NaqviHilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4**Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170)***Organized by:* K. Theopold, K. Mashima, Z. Xie
Presiding: K.H. Theopold**13:00 – 823.** Titanium tris-anilide cation: Discovery of a bis-titananoxyl carbene bonding mode for CO_2 and oxalate formation. A. Paparo, J. Silvia, H. Spinney, C. Clough, **C. Cummins***, T. Spaniol, J. Okuda, C. Kefalidis, L. Marion**13:30 – 824.** N_2 -splitting and functionalization in the coordination sphere of rhodium. **I. Klopsch**, C. Würtele, M. Finger, S. Schneider***13:50 – 825.** Tantallacarbonare-mediated cleavage of C-N multiple bond. **Z. Xie****14:20 – 826.** Construction of novel phosphorus functionalised carbynes of molybdenum and tungsten. **A.F. Hill***, A.L. Colebatch, R. Shang, A.C. Willis**14:40 – 827.** Zirconium-mediated activation of small molecules: Synthesis of functional carboranes. **Z. Qiu****15:00 – 828.** Paddlewheel Mo_2 -catalyzed hydrodehalogenation reaction of polyhaloalkanes. **H. Tsurugi**, S. Kando, R. Supriya, A. Hayakawa, Y. Sugino, K. Mashima***15:20 – 829.** Quintuple bond reactivity and high catalyst economy in coordinative chain transfer polymerization. **R. Kempe*****15:50 – 830.** Halogen exchange reaction of alkyl fluorides with organic halogen sources. **Y. Mizukami**, Z. Song, T. Takahashi***16:10 – 831.** Metal carbonyls as nucleophilic partners for frustrated Lewis pairs. **M. Sharma**, A.F. Hill*, N. Otten**16:30 – 832.** Activation of molecular nitrogen by early transition metal complexes. **M. Fryzuk***, A. YeoHilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2**Transition Metal Complexes of N-Heterocyclic and Mesoionic Carbenes: Structure, Materials and Catalytic Applications. (#195)***Organized by:* C. Cradden, S. Chang, M. Albrecht, D. Allen, U. Complete**13:00 – 833.** Transition metal complexes bearing carbenes beyond classical NHCs: Synthesis and catalytic activity. Y. Bidal, m. lesieur, M. Melaimi, f. nahra, G. Bertrand, **C. Cazin*****13:20 – 834.** Design of selective reactions of olefins. **R.H. Grubbs*****13:50 – 835.** Mono arylation of primary amines and ammonia using specially designed Pd-NHC complexes. R. Rucker, S. Sharif, N. Chandrasoma, D. Mitchell, M. Rodriguez, **M.G. Organ***, C. Lombardi**14:10 – 836.** Cationic 4-phosphonio-substituted NHCs and their coordination chemistry. **J.J. Weigand****14:30 – 837.** *N*-Heterocyclic olefins - a new class of tuneable ligands. **C. Hering-Jungjans**, K.C. Powers, E. Rivard***14:50 – 838.** Metal complexes of mesoionic carbenes: Electron reservoirs and catalysis. **B. Sarkar****15:10 – 839.** Enantiomerically pure bidentate amine tethered N-heterocyclic carbenes: Synthesis, transition metal complexes, and their asymmetric catalytic applications. **K. Wan**, H. Rebmann, A.J. Lough, R.H. Morris***15:30 – 840.** 3D structure determination of surface species by DNP enhanced solid-state NMR. **D. Gajan**, P. Berryer*, M. Lelli, A. Zagdoun, A. Rossini, M. Conley, O. Ouari, P. Tordo, C. Copéret, A. Lesage, L. Emsley**15:50 – 841.** Low-electron count platinum complexes stabilized by N-heterocyclic carbenes: From stoichiometric reactions to efficient catalysts. **S. Conejero****16:20 – 842.** Selective CH and CN bond activation on an iridium triazolylidene platform. **M. Albrecht***Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3**Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239)***Organized by:* K. Ishii, Z. Chen, P. Ford, G. Hanan**13:00** Opening remarks**13:05 – 843.** Toward controlling electron transfer in solution with bond-specific infrared excitation. M. Delor, P. Scattergood, M. Towrie, A. Parker, G. Greetham, T. Keane, I.V. Sazanovich, A. Meijer, **J.A. Weinstein*****13:30 – 844.** Synthesis of luminescent thiolato copper(I) complexes with bis-pyridyl ligands. **K. Tsuge**, T. Suzuki, M. Sato, H. Ohtsu, K. Nozaki**13:45 – 845.** Development of intelligent sensors based on Cu(I)-cluster luminesphore. **A. Kobayashi***, T. Hayashi, M. Yoshida, M. Kato**14:00 – 846.** Structural and photophysical diversity in d10 metal complexes. **T. Tsubomura****14:15 – 847.** Luminescent chromic metal complexes. **M. Kato*****14:40 – 848.** Insights into lanthanide sensitization using ultrafast spectroscopy. **E.G. Moore*****14:55 Coffee break****15:05 – 849.** Luminescent nanoparticles composed of lanthanide coordination polymers. **Y. Hasegawa*****15:20 – 850.** Interfacial europium complex on SiO_2 nanoparticles for reduction-induced blue light emission system. **A. Ishii***, M. Hasegawa**15:35 – 851.** Triarylboron-functionalized lanthanide complexes and their applications. J. Peng, T. Wu, **S. Wang*****15:50 – 852.** Detection of enzyme activities using luminescent lanthanide complexes. **T. Terai***, H. Ito, T. Nagano, Y. Urano***16:05 – 853.** Mixed transition-metal/lanthanide complexes as bifunctional imaging agents. **M. Ward*****16:20 – 854.** Phosphorescent rhenium complexes: New building blocks for metabolism trackers. **M. Massi***, M. Werrett, P. Wright, S. Plush, D. Brooks, S. Stagni**16:35 – 855.** Exploitation of the photophysical and photochemical properties of luminescent rhenium(I) and iridium(III) poly-pyridine complexes in the design of biological probes and photocytotoxic agents. **K. Lo****** Principle Author****Photographing of presentations and/or taping of talks is prohibited unless permission is obtained from the symposia organizers and individual presenters.****Final Pacificchem 2015 program online at:****<http://pacificchem.org/onlineprogram>**

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2

Inorganic Complexes for Solar Energy Harvesting (#256)

Organized by: M. Wolf, K. Sakai,
F. MacDonnell
Presiding: F.M. MacDonnell

13:00 Opening Remarks

13:05 – 856. Ultrafast photodriven redox processes in photocatalysts for artificial photosynthesis. **M.R. Wasielewski***, R. Lindquist, M. Majewski, W. Han, B.T. Phelan

13:40 – 857. Photoenergy conversion processes studied by time-resolved infrared spectroscopy. **K. Onda***

14:15 – 858. Electrochemical and excited-state properties of cyclometalated Ir(III)-Pt(II) and Ir(III)-Ir(III) bimetallic complexes bridged by dipyridylpyrazine. Y. Cho, H. Son, M. Baik, **S. Kang***

14:35 – 859. Ultrafast charge transfer across the 5-Pyridine/ZnO(10-10) interface. **J. Stähler***, J. Deinert, C. Richter, L. Bogner, M. Wolf

14:55 Break

15:10 – 860. Perspective of Karen Brewer's approach to solar fuel chemistry using supramolecular complexes. K.J. Brewer, **E.M. Naughton***, J.A. Beach, K.M. Felice, R.B. Moore

15:45 – 861. Photophysics of metal complexes with π -conjugated ligands. **M.O. Wolf**, M. Majewski, A. Howarth

16:05 – 862. Measurement of the activation energies of exciton migration in ruthenium(II) and rhodium(III) polypyridyl and phenanthroline complexes via luminescence at cryogenic temperatures. J.W. Kenney*, **G.A. Crosby**, P. Weaver, J. Macwillie

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

Metal Mediated Polymerization (#292)

Organized by: P. Hayes, R. Waterman, T. Mizuta, Y. Tang, P. Sangstriruthugul
Presiding: B. de Bruin, C.M. Kozak

13:00 – 863. Organolithium compounds for construction of olefin polymerization catalysts and for initiation of anionic styrene polymerization. **B. Lee***

13:30 – 864. Synthesis of cyclic olefin copolymers by half-titanocene catalysts. **w. zhao, K. NOMURA***

13:50 – 865. Characterization and mechanism of formation of the active site in the Phillip's ethylene polymerizatioin catalyst. **A.E. Stiegman**, S.L. Scott

14:10 – 866. Versatile approach to amine-containing polymers via tandem sequential hydroalkylation and ROMP. **L.L. Schafer***

14:40 Intermission

14:55 – 867. Synthesis of PE Oil, wax and UHMWPE by developing olefin polymerization catalysts. **X. Sun***, Y. Tang

15:25 – 868. Copolymerization of ethylene with methyl acrylate by bisphosphine monoxide-palladium catalysts enabled by ligand-controlled insertion regioselectivity. **Y. Mitsushige**, C. Brad P., S. Ito, K. Nozaki*

15:45 – 869. Copolymerization of polar monomers and α -olefins with late transition metal post-metallocene catalyst. **Y. Konishi**, N. Sato, K. Hirokane, H. Shimizu, H. Uchino, F. Shimizu, A. Tanna, T. Tayano

16:05 – 870. Extraordinarily active zwitterionic nickel catalysts for CO-ethylene alternating copolymerization. **L. Jia***

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Novel Heme Proteins and Model Systems (#305)

Organized by: J. Dawson, T. Hayashi, M. Stillman
Presiding: J. Dawson

13:00 break

13:40 – 871. Activation of cytochrome P450BM3 by decoy molecules for gaseous alkane hydroxylation. **O. Shoji***, Y. Watanabe*

14:00 – 872. Mechanisms of C-H oxygenation by heme-thiolate peroxigenases and related model systems. **J.T. Groves***

14:20 – 873. Capture and characterization of reactive intermediates in P450 catalysis: Insights into biological C-H bond activation. **M. Green**

14:40 – 874. Rerouting of cytochrome P450 ferryl intermediates for hydrocarbon biosynthesis. **T.M. Makris**

15:00 – 875. Light-driven P450 biocatalysts. **L. Cheruzel***

15:20 – 876. Vibrational coherence and kinetic studies of novel heme proteins. **P. Champion***

15:40 – 877. Effector role of pdx in P450cam studied by double electron-electron resonance. **D.B. Goodin***, S. Liou, X. Shi, M. Mahomed, X. Cheng, W. Myers, R. Britt

16:00 – 878. Controlled oxidation of aliphatic C-H bonds in recombinant P450 BM3: Mechanistic insights derived from studies on deuterated and fluorinated substituents. **S.S. Yu***, C. Yang, C. Lin

16:20 – 879. Heme porphyrin in NO synthase acts like a wire to deliver an electron at a specific step during catalysis. **D. Stuehr***

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Metal Coordination Sphere Design for Challenging Bond Transformations (#318)

Organized by: K. Caulton, A. Hill, S. Johnson, M. Yamashita

Presiding: S.A. Johnson, O.V. Ozerov

13:00 – 880. Bond cleavage by using low-coordinate group 9 metal complexes possessing a boron-based pincer ligand. **M. Yamashita***

13:20 – 881. Syntheses and reactions of new fused-ring metallobenzenes. B.J. Frogley, T.M. Christy, **L.J. Wright***

13:40 – 882. Chemoselectivity in activation of E-H and P-X bonds at late transition metals. **R.N. Perutz***, B. Procacci

14:00 – 883. N-Cleavage and functionalization by multinuclear iron systems. **K.C. MacLeod, P.L. Holland***

14:15 – 884. Oxidative addition to gold(I): It is all a question of ligand design. **A. Amgoune, D. Bourissou***

14:35 – 885. Amine oxidation mediated by iridium pincer complexes. **S. Schneider**

14:50 – 886. Palladium carbene complexes as persistent radicals. **V.M. Iluc***

15:05 – 887. Exploiting the redox activity of ligands with tetrazole functionality. **B. Cook, D. Skomski, R. Lord, A. Polozhaev, S.L. Tait, C. Chen, M. Pink, K. Caulton***

15:25 – 888. PCP pincer ligands anchored by carbene donors: M=C cooperative function in catalytic processes. **W.E. Piers***, L.E. Doyle, E. Lapierre, J.D. Smith, M. Sgro, D. Spasyluk

15:45 – 889. Macrocyclic platforms for small molecule redox chemistry: defining reaction space in di- and tetranuclear complexes. **J. Love***, J.R. Pankhurst, T. Cadenbach, M. Curcio

16:00 – 890. Controlling the reactivity of paramagnetic Group 10 metal complexes using flexible multidentate ligands. **L. Mirica***

16:15 – 891. Robust, ancillary ligand-free, catalysts of the first-row transition elements – hydrodesulfurization and hydrodeoxygenation under mild conditions. **J.M. Stryker**

16:30 – 892. Studies of the synthesis and reactivity of 2-nickelaoxetanes. **A. Desnoyer, E. Bowes, J. Love***

16:45 Flash Session 2

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Telomeres and other G-quadruplex Structures as Targets for Metallodrugs (#459)

Organized by: J. Aldrich-Wright, N. Sugimoto, J. Chaires, S. Ralph

Presiding: J. Aldrich-Wright, N. Sugimoto

13:00 – 893. Fifty shades of G: Quadruplexes come in many forms. **J. Mergny**

13:30 – 894. Binding interactions between nickel Schiff base complexes and DNA. **K.J. Davis***, C. Richardson, A. Willis, A. Guedin, J. Mergny, J.L. Beck, S.F. Ralph

13:50 – 895. Tetraplex nucleic acids in drug discovery and biosensing. **F. Shao***

14:20 – 896. G-quadruplex DNA interactions of dinuclear Pt(II) complexes. B. Harper, R. Vilar, N. Jones, S. Hoffmann, D.L. Ang, B.J. Pages, J. Aldrich-Wright*

14:40 Afternoon tea

14:55 – 897. Thioflavin T analogs as G-quadruplex indicators and their applications to bioanalysis. Y. Kataoka, H. Fujita, **M. Kuwahara***

15:15 – 898. G-quadruplex ligands toward photodynamic therapy. **D. Miyoshi***, K. Murata, H. Matsuno, N. Sugimoto

15:35 – 899. Assessment of the selectivity of Ni(II)-complexes towards G-quadruplex topologies. **A. De Rache***, L. Sabater, L. Lecarme, F. Thomas, G. Pratviel, J. Mergny

15:55 – 900. NMR insights into folding intermediates and novel tetrahedral G-rich structures. **J. Plavec**

16:25 – 901. Design and development of quadruplex-binding small molecules targeting human cancers. **S. Neidle***

Thursday Evening

Hawaii Convention Center
Halls I, II, III

Functional Nanomaterials Based on Coordination Chemistry (#73)

Organized by: T. Uemura, M. MacLachlan, H. Matsui

Poster Session

19:00 – 21:00

902. Efficient post-assembly modification of dynamic metallosupramolecular architectures. **D.A. Roberts**, J.R. Nitschke

903. Double-malate bridging tri-europium cluster encapsulated arsenotungstates with long-life luminescence. P. Ma, M. Imran, D. Zhang, J. Wang, **J. Niu**

904. Catalytic properties of metal-organic frameworks composited loading metal nanoparticles prepared through arc plasma deposition. **M. Sadakiyo***, S. Yoshimaru, H. Kasai, K. Kato, M. Takata, M. Yamauchi*

905. Modular assembly and guest-binding behavior of biomimetic coordination super-containers. **F. Dai***, Z. Wang, Z. Chen

906. Structural study of gold nanoparticles with sugar-type surfactant using SANS, SAXS, and XAFS methods. **K. Akutsu***, H. Iwase, Y. Nakatani, T. Yoshimura

907. Heteropentanuclear metal string complex $\text{Mo}_2\text{Ni}_2\text{Mo}_2$ with V-shaped quadruple bonds and a high spin square planar Ni(II) ion. **W. Hung**, G. Lee, S. Peng

908. Direct evidence of an equilibrium between tungsten (VI) alkyl-alkylidyne and its bis(alkylidene) tautomer through its reaction with surface N-donor ligands. **A. Bendjeriou-Sedjera***, J. Sofack-Kreuter, E. Abou-Hamad, K. Huang, J. Bassett

909. Fe(II)/Pt(II) based multifunctional heterometallo-supramolecular polymer. **C. Chakraborty***, S. Moriyama, M. Higuchi

910. Negative linear compressibility in a chiral coordination polymer. **H.H. Yeung***, A.K. Cheetham, S. Moggach

911. Synthetic, structural, and property analysis of a heterometallic Ni(II)/Cu(II) cage. **N.D. Shepherd***, F. Li, L.F. Lindoy, Y. Zhang

912. Phosphine-functionalized thiophene-based metallocopolymers. **J. Clifton***, I. Manners, P.G. Pringle

913. Characterization for metal-oxide nanoparticles generating radicals with X-ray irradiation. **C. NUMAKO***, S. Miyazaki, K. Sato, S. Takami, C. Ogino, A. Kondo

914. Structural control of chloranilamine-based hybrid compounds. **K. Kanazashi**, R. Ishikawa, S. Kawata

915. DNA aptamer interactions with aqueous gold interfaces: Influences of interfacial shape, presence of citrate, and temperature on structure disorder. **K.L. Drew**, Z.E. Hughes, J. Palafax-Hernandez, T.R. Walsh

916. Direct synthesis and evaluation of complexes in an inner aqueous phase of liposome. **M. Honjo***, T. Koshiyama, M. Ohba

917. Metal-to-metal charge transfer and spin-crossover in mixed-valence iron coordination polymers. **K. Nakamura**, S. Kang, S. Kanegawa, O. Sato

918. Building block approach in the design of coordination polymers based on metal-pyrazinediol complexes. **M. Ogawa**

919. Velocity visualization of rotational motions in a dirhodium-centered, circularly-arranged four-gear system. **K. Sanada**, H. Ube, M. Shionoya*

920. Controlled radical copolymerization of vinyl monomers in a porous metal complex with coordinatively unsaturated sites. **S. Mochizuki**, T. Uemura, S. Kitagawa

921. Reversibly electroswitchable photoluminescence using Fe(II)-based metallo-supramolecular polymer. **T. Suzuki***, T. Sato, J. ZHANG, M. Higuchi, H. Maki

922. Ferroelectric coordination polymers self-assembled from liquid crystalline zinc(II) porphyrin and dipyridyl ligands. **J.K. Hui**, H. Kishida, K. Takemasu, M. Morikawa, N. Kimizuka*

923. Synthesis of human serum albumin having a terpyridyl group and its dimer formation by metal-coordination. **S. Suzuki**

924. Design of novel inorganic-organic hybrids constructed from chloranilic acid and n-alkylamine. **S. Yagisita**, S. Kawata, R. Ishikawa, A. HIMEGI

925. Syntheses and properties of planar-typed complexes bridged by TCNQ derivatives. **S. Ueno**, R. Ishikawa, S. Kawata

926. Stepwise regioselective quarter sphere hexa-imidization of $[\text{Mo}_3\text{O}_{19}]^{2-}$, $[\text{Mo}_3\text{W}_{10}]^{2-}$, $[\text{Mo}_3\text{V}_{12}]^{2-}$ by applying $[\text{Mo}_3\text{O}_7(\text{NAr})_3](\mu_2\text{-NAr})_3$ as a structure-directing template. **J. Zhang**, Y. Huang, J. Hao, Y. Wei

927. Synthesis and structure of ladder-type Pd-halide chain complex. **R. Kimura**, S. KUMAGAI, H. Iguchi*, S. Takaishi, M. Yamashita*

928. Syntheses and characterizations of tiara-shaped metal-thiolate macrocyclic hosts. **Y. Shichibu***, K. Yoshida, K. Konishi

929. Formation of sub-micron coordination particles using a phosphonate ligand. **K.J. Bladet**, B. Gelfand, G. Shimizu

930. Helical metalloc-supramolecular polymer and their DNA binding and cytotoxicity study. **U. Rana***, M. Higuchi

931. Ionic conductivity of metalloc-supramolecular polymers having linear and 3D structure. **R.K. Pandey***, T. Sato, M.D. Hossain, S. Moriyama, M. Higuchi

* Principle Author

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- 932.** Control of coordination bond angles in $[\text{Mn}^{\text{V}}(\text{NCN})_4]^{2-}$ using dabco- $(\text{CH}_2)_{x-1}\text{-CH}_3$ cations ($x=15\sim18$) and parity effect on the redox potentials. **Y. Kitamura**, R. Ohtani, K. Takami, m. nakamura, S. Hayami
- 933.** Metal-directed short peptide folding and assembly for unique entangled nanostructures. **T. Sawada**, A. Matsumoto, M. Yamaguchi, M. Fujita*
- 934.** Large indium-selenide triangular ring cluster: Structure and templating effect. **J. Dai***, Q. Zhu*, Y. Wang
- 935.** Fabrication and its diode behavior of heterolayer film composed of the Ru complex and Prussian blue nanocrystals. **H. SATO**, H. Ozawa, K. Kanazuka, M. Kurihara, M. Haga*
- 936.** Synthesis and guest encapsulation of sugar sponge. **G. Ning**, Y. Inokuma, M. Fujita*
- 937.** Nanosized neutral luminescent organometallic macrocycles based on Ir(III) porphyrin: From controlled self-assembly to optical functional supramolecules. **L. Qin**, C. Che
- 938.** Polysilane confined in coordination nanospaces. **T. Kitao***, T. Uemura, S. Kitagawa
- 939.** Synthesis and structural determination of metal directed julolidine based optical sensors. **D.J. Fanna***, F. Li, J. Reynolds
- 940.** Synthesis of porphyrin wire connected by Pd(II) coordination. **Y. Yagisawa**, Y. Yamazawa, T. Komatsu*
- 941.** Mixing of immiscible polymers using nanoporous coordination templates. T. Uemura*, T. Kaseda, **Y. Sasaki**, S. Kitagawa
- 942.** Structural control of crystalline folded peptide coordination networks. **M. Yamagami**, T. Sawada, M. Fujita*
- 943.** Large spin-crossover $[\text{Fe}_4\text{L}_4]^{8+}$ tetrahedral cage. L. Li, L.F. Lindoy, C. Li, J. Aldrich-Wright, F. Li

Hawaii Convention Center
Halls I, II, III

Coordination and Supramolecular Chemistry for Aqueous Metal Ion Separations (#97)

Organized by: R. Ellis, D. Robinson, R. Motokawa

Poster Session 19:00 – 21:00

- 944.** Separation and recovery of rare metal ions from saline water using synthetic peptides. **T. Jung**, D. Pamidimari, S. Hong, S. Jeon, S. Chung, J. Na*
- 945.** From molecular coordination to supramolecular structure of organic phases: Multiscale experimental and theoretical studies. **G. Ferru***
- 946.** Sulfonamide extractants and analogs in separations and sensing applications: Combining coordination chemistry and solvent extraction principles for designing selective extractants and sensors for toxic metals and other ionic targets. **K. Kavalieratos***
- 947.** Effect of metal salts on the oxidation reaction of (acetylphenyl)ferrocenes. **S. Yamamoto***, Y. Okada
- 948.** Understanding actinide and lanthanide complexation in solution: From fundamentals to applications. **P.V. Dau**, Z. Zhang, L. Rao*
- 949.** Progress towards new calix[4]arene based stationary phases useful in the separation of rare earth metals. **S.R. Menon**, J.A. Schmidt*
- 950.** Coordination ability of 1,1'-disubstituted ferrocenes bearing pyridyl group. **M. Murayama***, Y. Okada
- 951.** Coordination ability of 1,1'-disubstituted ferrocenes bearing ethyleneoxy chain. **T. Morita***, Y. Okada

Hawaii Convention Center
Halls I, II, III

Frontiers of Molecular Magnetism (#109)

Organized by: H. Oshio, J. Miller, R. Oakley, S. Brooker, S. Gao, M. Ohba

Poster Session

19:00 – 21:00

- 952.** Cyanide-bridged Co–W bimetal assembly exhibiting photo-induced charge transfer phase transition at room temperature. **Y. Miyamoto***, N. Ozaki, Y. Umetsu, K. Imoto, T. Tokoro, K. Nakabayashi, S. Ohkoshi
- 953.** Spatially inhomogeneous, stepwise phase transitions in a heterocyclic thiacyl diradical: Geometrical frustration induced by mismatch between translational symmetry and lattice transformation. **R. Suizu**, Y. Shuku, K. Awaga
- 954.** 2,5-Disubstituted transition metal 1,3,4-oxadiazoles for spin crossover compounds. **C. Köhler**, E. Rentschler*
- 955.** Research for the relationship between structure and spin crossover phenomena in new type of iron(III) dithiocarbamate complex. **T. Yamabayashi**, K. Kagesawa*, B.K. Breedlove, M. Yamashita*
- 956.** NO responsivity of a Hofmann-type porous coordination polymer and magnetic behavior of its NO clathrate. **A. Mishima**, R. Ohtani, A. Horii, R. Matsuda, S. Kitagawa, T. Koshiyama, M. Ohba*
- 957.** Mononuclear and polynuclear spin-crossover iron(II)-bis(pyrazol-1-yl)pyridine complexes. **I. Salitros***
- 958.** Synthesis, structure, and SMM behavior of a $\text{Zn}^{(\text{II})}\text{-Ce}^{(\text{III})}\text{-Zn}^{(\text{II})}$ complex with pseudo threefold symmetry. **N. Irie**, S. Kayahara, H. Wada, S. Ooka, C. Takehara, P. Then, Y. Kataoka, T. Kajiwara, T. Yamamura
- 959.** Fe(II) spin crossover complexes with hexadentate tripodal ligands derived from 1R,2,3-triazole-4-carbaldehyde and tris(2-aminoethyl)amine. **R. Minoura**, H. Hagiwara*
- 960.** Linear two-coordinate transition metal complexes: Potential candidates for single molecule magnets?. **C. Lin***, P.P. Power
- 961.** Spin transition behavior of mixed-metal porous magnetic solid solution. **M. Tsuji**, A. Mishima, Y. Ohtsubo, T. Koshiyama, M. Ohba*
- 962.** Magnetic property and optical property of cesium manganese pentacyanidonitrosomolybdate assembly. **M. Komine**, K. Imoto, Y. Miyamoto, K. Nakabayashi, S. Ohkoshi
- 963.** Pushing the limits of magnetic anisotropy in monometallic 3D single-molecule magnets. K.E. Marriott, L. Bhaskaran, C. Wilson, R.J. Deeth, S.T. Ochsenbein, S. Hill, M. Murrie*
- 964.** Effect on the ferromagnetic transition temperature of the cobalt layered hydroxides by employment of the monovalent diarylethene derivative with a carboxyl group. **Y. Inada**, S. Kubota, A. Okazawa, N. Kojima, M. Enomoto
- 965.** Study of single-chain magnet-like behavior in $(\text{NH}_4)_2\text{MnF}_5$. **J. Satoh**, K. Kagesawa*, S. Takeishi, B.K. Breedlove, M. Yamashita*
- 966.** High-spin ground state and single-molecule magnet behavior in tri- and hexanuclear iron clusters. **R. Hernández Sánchez**, G. Ménard, T. M. Powers, T. Bettley*
- 967.** Magnetic properties of hydroxyl-bridged heptanuclear complexes. **Y. Tsuji***, T. Togo, A. Mishima, T. Koshiyama, M. Ohba
- 968.** Optical bistability in a photochromic valence tautomeric cobalt cluster. **A. Kurimoto**, M.M. Paquette, N.L. Frank
- 969.** Spin-crossover FeIN6 complexes of nonplanar tridentate ligands: An overview. **S. Javed***
- 970.** Multistep phase transition in cyanide-bridged multinuclear complexes. **M. Nihei***, Y. Yanai, H. Oshio
- 971.** High ionic conductivity on cyano-bridged metal assemblies. **K. Nakagawa**, K. Imoto, S. Ohkoshi
- 972.** Synthesis and characterization of a new air stable 1,2,4-triazinyl radical and its coordination complexes. I.S. Morgan, A. Mansikkämäki, P. Koutentis, R. Clerac, H.M. Tuunonen*
- 973.** Hysteretic spin crossover with remarkable shift of critical temperature in new iron(II) complexes with 1,2,3-triazole containing tetradeятate ligand. **S. Okada**, H. Hagiwara*
- 974.** Magnetic properties of dysprosium(III)-yttrium(III) phthalocyaninato quadruple-decker complexes. **Y. Horii**, K. Katoh, B.K. Breedlove, M. Yamashita
- 975.** Insufficiency of the anisotropy barrier, as the sole criterion, for the design of lanthanide single-molecule magnets. **K.S. Pedersen***, J. Bendix, J. Dreiser, M. Soerensen, R. Sibile, H. Mutka, S. Piligkos
- 976.** Photoinduced magnetization in spin-crossover Fe- $[\text{Nb}(\text{CN})_6]$ -based assembly. **K. Imoto**, H. Tokoro, S. Ohkoshi
- 977.** Reactivity of novel diiron complex with anthracene framework. **K. Fujimoto**, T. Suzuki, T. Inomata, T. Ozawa, H. Masuda, M. Fryzuk
- 978.** Syntheses and SMM behaviors of lanthanide(III) azacrown-ether complexes: Correlation between magnetic behaviors and crystal structures. **H. Wada***, S. Ooka, P. Then, C. Takehara, Y. Kataoka, T. Kajiwara, T. Yamamura
- 979.** Magnetic properties of Co^{2+} ion doped Hofmann-type spin-crossover complex: $\text{Fe}_{1-x}\text{Co}_x(3\text{-Fluoropyridine})_2[\text{Au}(\text{CN})_2]$. **S. Matsumoto***, J. Okabayashi, T. Kitazawa
- 980.** Structures and magnetic properties of a series of Ln_4 tetrahedral complexes: A Dy analog with single-molecule magnet behavior. **H. Tsai**, P. Huang
- 981.** Tuning interchain interaction by ligand manipulation in 2D network assembled with Mn(III) Schiff-base complex and dicarboxylic acids. **K. Kagesawa***, y. aono, h. yoshida, K. Katoh, B.K. Breedlove, M. Yamashita*
- 982.** Magnetic and guest adsorption properties of porous magnets having dianion-based pseudo-pillared-layer type structure. **N. Tomokage***, H. Miura, A. Mishima, T. Koshiyama, M. Ohba
- 983.** Two Gd^{3+} coordination polymers derived from flexible dicarboxylate ligands as attractive cryogenic magnetorefrigerants. **S. Liu**, T. Zheng, H. Wen
- 984.** Proton-induced switching of the SMM properties of a terbium(III)-phthalocyaninato double-decker complex. **Y. Horie**, Y. Horii, K. Katoh, B.K. Breedlove, M. Yamashita
- 985.** Single ion magnets with multiple relaxation processes based on Co(II) and Ni(II) complexes. **R. Boca**
- 986.** Syntheses and magnetic properties of transition-metal complexes with multichelating and high-spin radical ligands. **A. Okazawa***, T. Ishida, N. Kojima, K. Ogawa
- 987.** Hydrogen adsorption and ortho-para conversion in porous magnets. **Y. Ohtsubo**, A. Mishima, A. Horii, T. Koshiyama, S. Kitagawa, M. Ohba
- 988.** Magnetometry on nanoscale iron-oxide deposits in the human brain. **L. Dihan***, M. Kopani, R. Boca
- 989.** Correlation between charge transfer on a magnetic layer of the iron mixed valence complex and molecular polarization of cationic intercalants. K. Arai, H. Ida, A. Okazawa, N. Kojima, M. Enomoto
- 990.** Magnetic properties of π -stacked pillarared layer framework complexes with intercalated $[\text{MCP}_2]^+$. **H. Fukunaga**, Y. Sekine, W. Kosaka, K. Taniguchi, H. Miyasaka*
- 991.** Effect of the direction of naphthalene moiety in $[\text{Fe}(\text{sal}-\text{Cl})_2]$ system. **Y. Norifumi**, T. Okubo, M. Maekawa, T. Kuroda-Sowa
- 992.** Synthesis and physical properties of a cyanide-bridged Fe-Co cage complex. **R. Wei**, T. Shiga, G.N. Newton, H. Oshio*
- 993.** Bis(tridentate) Schiff-base bridged spin transition iron complexes using "click" chemistry. **H. Hagiwara***, T. Tanaka, S. Hora
- 994.** Crystal structures and physical properties of electron accepting thiadiazole dioxide compounds and their transition metal complexes. **Y. Shuku**, K. Awaga*
- 995.** Modulation of magnetic dynamics of Dy-complexes driven by crystal packing. **M. Kamilla***, G. Cosquer, M. Yamashita
- 996.** Strongest ferromagnetic exchange coupling in gadolinium(III)-nitroxide coordination compounds. **T. Kanetomo***, T. Yoshitake, T. Ishida
- 997.** Effect of the hydrogen-bond network in $[\text{Fe}(\text{sal}-\text{Cl})_2]$ spin crossover system. **T. Kuroda-Sowa***, A. Hinano, K. Sugimoto, T. Okubo, M. Maekawa
- 998.** Counter-ion effects on magnetic properties of dicarboxylate-bridged $[\text{Mn}(\text{salen})]$ complexes having two-dimensional network structure. **Y. Nishimura**, h. yoshida, B.K. Breedlove, K. Kagesawa*, M. Yamashita*
- 999.** Syntheses and SMM behaviors of linear $\text{Zn}^{(\text{II})}\text{-Ln}^{(\text{III})}\text{-Zn}^{(\text{II})}$ trinuclear complexes with pseudo threefold symmetry ($\text{Ln} = \text{Pr}, \text{Nd}$). **S. Kayahara***, N. Irie, S. Ooka, H. Wada, C. Takehara, P. Then, Y. Kataoka, T. Kajiwara, T. Yamamura
- 1000.** Crystal structures and magnetic properties of photoresponsive 2p-4f heterospin complexes. **K. Murashima**, S. Karasawa*, N. Koga*
- 1001.** Synthesis, crystal structure, and magnetic properties of the face-shared triply bridged linear trinuclear complexes. **Y. Sunatsuki***, T. Kobayashi, T. Fujino, M. Iwayama, M. Kojima, T. Suzuki, N. Matsumoto, N. Re
- 1002.** Magnetic properties of heterospin single-molecule magnets (SMMs) in frozen solution: Roles of S_{total} value in SMMs. **S. Karasawa***, K. Nakano, D. Yoshihara, J. Tanakashira, N. Yamamoto, T. Yoshizaki, Y. Inagaki, N. Koga*
- 1003.** Chirality-assisted preparation of hetero metallic complexes and their physical properties. **S. Kanegawa**, S. Kang, O. Sato
- 1004.** Unexpected, cooperative spin-cross-over in iron(III)/dipyrazolylpyridine complexes with large Jahn-Teller distortions. L.J. Kershaw Cook, R. Kulmaczewski, G. Chastanet, T.P. Comyn, M.A. Halcrow*
- 1005.** Reversible photomagnetic effect on $\text{FeNb}\text{-octacyano}$ bimetal assembly. **H. Tokoro***, K. Imoto, S. Ohkoshi*
- 1006.** Preparations, molecular structures, and magnetic properties of photoresponsive cyclic dinuclear $\text{Mn}^{(\text{II})}\text{-Fe}^{(\text{II})}\text{-Ni}^{(\text{II})}$ complexes in heterospin systems. **K. Mori**, D. Yoshihara, S. Karasawa*, N. Koga*

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170)

Organized by: K. Theopold, K. Mashima, Z. Xie

Presiding: J. Arnold

19:00 – 1007. Catalytic alkyne and diyne metathesis. **M. Tamm**

19:30 – 1008. Group 4 metal complexes containing amine/phosphine biphenolate ligands: Structure and catalysis. **L. Liang***

20:00 – 1009. Synthesis of the well-defined silica supported molybdenum-catalyst for metathesis of n-decane. **J. Bassett**, S. Kavitate, M. Samantaray, R. Dey

* Principle Author

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20:30 – 1010. Sidearm approach to catalysts for olefin polymerization: Controllable synthesis of polyethylene. **Y. Tang**

Hawaii Convention Center
Halls I, II, III

Transition Metal Complexes of N-Heterocyclic and Mesoionic Carbenes: Structure, Materials and Catalytic Applications. (#195)

Organized by: C. Crudden, S. Chang,
M. Albrecht, D. Allen, U. Complete

Poster Session
19:00 – 21:00

1011. Dinick(II) complexes bearing bulky NHC ligand as catalysts in the Kumada-Tamao-Corriu coupling of aryl halides. **K. Matsubara***, Y. Koga, K. Nonaka, T. Inatomi

1012. Carbene complexes with main group element and transition metal halides: Syntheses and applications. **G. Roessenthaler***, T. Boettcher, L. Lewis-Alleyne

1013. Exploring new ligand architectures for ruthenium-mediated olefin metathesis. **G. Lavoie***, T. Larocque, A. Badaj

1014. Pincer complexes with central N-heterocyclic carbene donor for small molecule activation. **Y. Jiang**, R. Roesler*

1015. Homo- and hetero-bimetallic coinage metal N-heterocyclic carbene complexes. **P.J. Barnard**

1016. Application of open chain tetraimidozolium ruthenium-NHC complexes in catalysis. **M. Hollering***, C. Jandl, A. Pöthig, F. Kuhn

1017. Palladium-catalyzed asymmetric allylic alkylation using C_2 -symmetric chiral bis(N-heterocyclic carbene) ligands. **Y. Yamaguchi***, Y. Suzuki, M. Asami

1018. Saturated N-heterocyclic carbenes-Pt complexes: Synthesis and catalytic activity for olefin hydrosilylation. **B. Yoo***, J. Han

1019. Dehydrocoupling of amine-boranes catalyzed by cyclometalated-NHC iron complex: Isolation of intermediate borato complexes and reaction kinetics. **H. Takahashi**, T. Watanabe, H. Tobita*

1020. Nickel-catalyzed alkynylation of anoles via carbon-oxygen bond cleavage. **M. Tobisa***, T. Takahira, N. Chatani

1021. Synthesis and reactivities of pincer-type complexes bearing protic N-heterocyclic carbene and pyrazole. **T. Toda**, S. Kuwata*, T. Ikariya

1022. Enantioselective Rh-catalyzed addition of arylboronic acids to aldehydes using NHC ligands bearing a cyclodextrin. **S. TSUDA**, K. ASAHI, T. Iwasaki, S. Fujiwara, H. Kuniyasu, N. Kambe

1023. Control of *cis*-selectivity and tacticity in ring-opening metathesis polymerization. **L. Rosebrugh**, V. Marx, T. Ahmed, J. Hartung, R.H. Grubbs*

1024. Synthesis, structures, and photoluminescence of pincer type C⁴C⁵N-heterocyclic carbene platinum(II) complexes. **J. Liu**, C. Che*

1025. Imidazo[1,5-*a*]pyridine carbene: Synthesis and characterization of annulated N-heterocyclic carbenes. **Y. Koto***, F. Shibahara, T. Murai

1026. Syntheses and catalytic ability of palladium complexes with sugar-incorporated N-heterocyclic carbene pincer ligands. **Y. Imanaka**, H. Hashimoto, T. Nishioka*

1027. Buchwald-Hartwig amination of aryl halides catalyzed by Ni(II) complexes and studies on the reaction mechanism. **T. Inatomi**

1028. Synthesis and structure of gold complexes using macrocyclic N-heterocyclic carbene ligands. **K. Fukasawa**, T. KATO, N. NISHINA*

1029. Proton induced generation of remote N-heterocyclic carbene–Ru complexes. **T. Fukushima***, K. Kobayashi, K. Tanaka

1030. Synthesis and structure of gold complexes using alkyne substituted N-heterocyclic carbene ligands. **E. Hasegawa**, N. NISHINA*

1031. Utilization of (η^6 -arene)Ni(*N*-heterocyclic carbene) complexes as a precursor of Ni(0) source. **Y. Hayashi**, Y. Hoshimoto, M. Ohashi, S. Ogoshi*

1032. Bi and trimetallic gold complexes of diphenylphosphinoethyl-functional imidazolium salts and their *N*-heterocyclic carbenes: Synthesis and photophysical properties. **S. Bestgen**

1033. Nickel-catalyzed reductive cleavage of anisole derivatives in the absence of external reductant. **M. Tobisa***, **T. Morioka**, N. Chatani

1034. Atmospheric CO₂ fixation using ruthenium complexes having a CNC-type pincer ligand. **T. Nakamura**, S. Ogushi, E. Kazushige, Y. Arikawa, K. Umakoshi

Hawaii Convention Center
Halls I, II, III

Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239)

Organized by: K. Ishii, Z. Chen, P. Ford, G. Hanan

Poster Session
19:00 – 21:00

1035. Synthesis of bacteriochlorophyll-*d* amino-analogs and their self-aggregation. **H. Watanabe***, S. Shoji, T. Mizoguchi, H. Tamiaki

1036. Circularly polarized luminescence in lanthanide(III) complexes having a chiral bis(oxazoline) pyridine ligand and its application. **J. Yuasa**, K. Uemura, T. Kawai

1037. Very long-lived photoinduced charge-separated states of triphenylamine-naphthalenediimide dyads in rigid media.

K. Kimoto*, T. Satoh, K. Nozaki, M. Iwamura, T. Horikoshi, S. Suzuki, M. Koizaki, K. OKADA

1038. Luminescence properties and anion sensing with Ln(III) complexes containing pybox ligands. **Y. Kataoka***, M. Harai, I. Tomotsuka, S. Shinoda, T. Kajiwara

1039. Advances in optical imaging through the design, synthesis, and fundamental investigation of phosphorescent metal tetrazolate complexes. **M. Werrett**, M. Massi, P. Rigby, S. Muzzoli, S. Stagni

1040. Theoretical study on metal–arene interaction for modulating light absorption and fluorescence. **M. Sugimoto***

1041. Temperature and pressure dependences of flexible cube-like framework in crystalline state: Structure and luminescent properties of [Ag₄₄(P_{p-tol})₄]**M. Nishiyama**, Y. Ozawa*, Y. Akahama, K. Toriumi, M. Abe

1042. Photoexcited state energy transfer of dual-emission in cube-like tetranuclear copper(I) halide complexes. **S. Nagaoka***, S. Yamasaki, Y. Ozawa, K. Toriumi, M. Abe

1043. Chiral sensing of amino acids in water using circularly polarized luminescence from achiral rare-earth complexes. **M. Iwamura***, T. Uchida, K. Nozaki

1044. Synthesis and optical properties of a bimetallic complex with a [7]helicene ligand. **M. Akiyama**, Y. Tsuchiya, A. Ishii, M. Hasegawa, K. Nozaki*

1045. Tuning the excited state of water-soluble iridium(III)-based DNA intercalators for the construction of optical probes. **S. Stimpson***, J. Thomas

1046. Synthesis and photochemical properties of BODIPY-imino oligomers. **M. Tsuchiya**, R. Sakamoto*, H. Nishiura*

1047. Photophysical and redox properties of copper(I) complexes and their oxygen responsive luminescence in the solid state. **M. Nishikawa**, T. Tsubomura*

1048. Photocatalysis of transition metal complexes for production of hydrogen peroxide from water and dioxygen utilizing water oxidation catalysts. **Y. Isaka**, K. Oyama, T. Suenobu, Y. Yamada, S. Fukuzumi*

1049. Electrochemically-controlled photophysical properties of both emission and coloration by luminescent lanthanide(III) complex and viologen derivatives. **K. Nakamura***, K. Kanazawa, Y. Komiya, N. Kobayashi

1050. Photophysical properties of lanthanide clusters with closed Ln-O lattice. **T. Nakaniishi***

1051. Photon upconversion based on triplet-triplet annihilation upconversion from near-IR to visible region using metal phthalocyanines. **J. You**, F. Zhang, J. Han, T. Morifumi, H. Yonemura*, S. Yamada, X. Li*, S. Wang, Y. Xiao

1052. Synthesis and photophysical properties of novel metal complexes having arylborane units. **E. Sakuda***, Y. Kanno, K. Takaki, A. Ito, N. Kitamura, S. Horuchi, Y. Arikawa, K. Umakoshi*

1053. Face-capping and terminal ligands effects on excited triplet states of octahedral hexamolybdenum clusters: (⁷Bu₄N)₂[Mo₆O₁₄Y₆] (X = halogen, Y = halogen). **S. Akagi***, N. Kitamura

1054. Near-UV emitting phosphorescent gel of iridium(III) complexes. **N. Darmawan***, L. De Cola*

1055. Molecular pin boards as optical sensors for biomolecules. **T. Andrews**, J. Thomas, G. Leggett

1056. Ruthenium(II) metallo-intercalating complexes conjugated to nanoparticle materials as novel probes for DNA. **S.J. Ashworth***, J. Thomas

1057. Mono and dinuclear complexes as anticancer therapeutic leads. **P.J. Jarman**, J. Thomas*

1058. Luminescence anion sensing with mixed-Ln(III) complex containing tridentate pybox ligand. **K. Nakamura***, M. Nokami, I. Tomotsuka, M. Harai, Y. Kataoka, T. Kajiwara

1059. Chromotropism of hydro-bridged dinuclear rhodium(III) complexes containing a tripodal tridentate phosphine ligands. **M. Kashihara**, T. Suzuki, Y. Sunatsuki

1060. Synthesis and photophysical properties of platinum complexes having arylborane units. **s. miyoshi**, E. Sakuda, A. Nakamura, N. Kitamura

1061. Synthesis and valence tautomerism of cobalt complexes with a dioxolene ligand containing a π -conjugated system. **K. Katayama**, M. Hirotsu*, I. Kinoshita, Y. Teki*

1062. Synthesis and excited-state characteristics of novel tricarbonyl rhodium(I) complexes having multiple arylborane charge transfer units. **Y. Kang***, A. Ito, E. Sakuda, N. Kitamura

1063. Synthesis of novel dicationic pyrene derivative and photochemical properties of the pyrene/clay hybrids. **D. Morimoto**, K. Sato, K. Saito, M. Yagi, T. Yui

1064. Electrochemical analysis of photoaction of metal complexes in solution. **A. Fukatsu**, M. Okamura, Y. Okabe, M. Kondo, S. Masaoka*

1065. Synthesis of a bridging ligand with dual metal binding sites and multistep assembly with zinc(II) ion. **Y. Imai**, J. Yuasa, T. Kawai

1066. Optical resolution of *cis*-Ru(bipy)₂(CN)₂ and photoinduced racemization of enantiomer. **Y. Alihara**, K. Sato, K. Shinozaki*

1067. Enhancement of MLCT absorption and phosphorescence of polyppyridyl ruthenium(II) complexes based on arylborane substituent. **A. Nakagawa**, E. Sakuda, A. Ito, N. Kitamura*

1068. Organometallic copper luminophores supported by a series of tridentate ligands. **Y. Kim**, S. Ahn, J. Kim, S. Kim, Y. Lee*

1069. Characteristic luminescent properties of seven-coordinated lanthanide complexes. **K. Yanagisawa**, T. Nakanishi, Y. Kitagawa, T. Seki, H. Ito, K. Fushimi, Y. Hasegawa*

1070. Luminescent mechanochromic system of silver(I) complexes containing diphenophanes bridged by aromatic groups. **T. Tsukuda**

1071. Photocatalytic CO₂ reduction using Cu and Fe complexes. **H. Takeda**, O. Ishitani*

1072. Luminescence/quenching properties in solutions and in the solid state of lanthanide complexes with tridentate ligand based on intermolecular interaction. **Y. Tsuchiya***, A. Ishii, M. Hasegawa

1073. Oxidation chemistry of metal(II)-diphenolato complexes with salen-type ligands: Electronic structure and reactivity relationship. **Y. Shimazaki**

1074. Physical properties of synthetic chlorophyll derivatives possessing a sulfur-functional group. **K. Kim**, H. Tamiaki

1075. Photophysical and magneto-optical properties of nonanuclear Tb(III) clusters with chiral ligands. **S. Wada**, Y. Kitagawa, T. Nakaniishi, K. Fushimi, Y. Morisaki, K. Fujita, K. Konishi, K. Tanaka, Y. Chujo, Y. Hasegawa*

1076. Effective photosensitized energy transfer of nonanuclear terbium clusters using methyl salicylate derivatives. **S. Omagari***, T. Nakaniishi, Y. Kitagawa, T. Seki, Y. Takahata, K. Fushimi, H. Ito, Y. Hasegawa

1077. CO₂ photoreduction based on Ru(II) complex having triarylborane unit. **N. Ishizaki***, E. Sakuda, N. Kitamura

1078. Monolithic devise for solar CO₂ reduction using H₂O by semiconductor/metal-complex hybrid photocatalyst. **S. Sato**, T. Arai, T. Morikawa

1079. Syntheses of phosphorescent iridium complexes with tridentate 3(5)-substituted pyrazole ligands. **T. ODAKA**, H. Ozawa, M. Haga*

1080. Synthesis and photochemical properties of new 2-aminophenolato complexes. **R. Tanaka**, M. Wakizaka, T. Matsumoto, H. Chang*

1081. Faraday effects based on 4f-4f transitions depending on the lanthanide ion and crystal field of the complexes. **Y. Kitagawa***, S. Wada, T. Nakanishi, K. Fushimi, Y. Hasegawa

1082. Photoactivation of single molecule magnet behavior in manganese-based complex. **A. Feto***, G. Cosquer, M. Morimoto, M. Irie, M. Yamashita

1083. Photoactivated NO-releasing Ru(ebp-p)(NO) complexes. **M. Kim**, h. Lee*

1084. Highly luminescent thulium complex of a hexadentate ligand with long alkyl chains. **K. Kuroda***, K. Sugimoto, A. Ishii, M. Hasegawa

1085. Luminescent Eu(III) coordination polymers cross-linked with transition metal ions. **M. Yamamoto***, T. Nakanishi, Y. Kitagawa, T. Seki, H. Ito, K. Fushimi, Y. Hasegawa

1086. Syntheses and luminescence properties of Ln(III) complexes containing pentadentate pybox derivative. **M. Nakami***, K. Nakamura, I. Tomotsuka, M. Harai, Y. Kataoka, T. Kajiwara

1087. Circularly polarized luminescence from Pt(N⁺C⁺N⁺X) excited-dimer + trimer having chiral ligand. **S. Tanaka***, K. Sato, T. Tsubomura, K. Shinozaki

1088. Shape-memory platinum(II) complex: Intelligent sensor for vapor, pressure, and temperature. **Y. Shigeta***, M. Yoshida, A. Kobayashi, M. Kato

1089. Efficient photocatalytic CO₂ reduction involving a CO₂-capturing Re(I) complex. **T. Morimoto***, O. Ishitani

1090. Synthesis and luminescence of copper(I) complexes bearing a diphosphine dioxide ligand. **T. Nishi**, M. Nishikawa, T. Tsubomura*

1091. Ratiometric optical sensors based on dual emission of a blue fluorescent coumarin and a red phosphorescent cationic iridium(III) complex for oxygen sensing in living cells. **T. Yoshihara***, S. Tobita

* Principle Author

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<http://pacifichem.org/>

onlineprogram

- 1092.** Synthesis and photophysical property of supramolecular complexes with platinum(II) organometallics including two pyridine units as metalloligands.
M. Shiotsuka*, Y. Itou, T. Toda, K. Sako
- 1093.** Crystal structures and photophysical properties of cyclometalated platinum(II) complexes drastically controlled by a carboxy group.
M. Ebina, M. Yoshida, A. Kobayashi, M. Kato
- 1094.** Chiroptical properties of Pd(0) complexes bearing chiral diphosphine ligands.
Y. Yamada, M. Nishikawa, T. Tsubomura*
- 1095.** Oxygen-dependent emission of copper(II) complexes bearing fluorinated diphosphine and phenanthroline ligands.
M. Washimi, M. Nishikawa, T. Tsubomura*
- 1096.** Triplet excimer formation and ciroptical properties of platinum(II) complexes bearing 2-phenylpyridine and chiral β -diketonate ligand.
j. morikubo, M. Nishikawa, T. Tsubomura*
- 1097.** Syntheses of macrocyclic tetranuclear ruthenium complexes by self-assembly and light-harvesting photoreaction of guest molecules in the cavity.
S. Shibata, M. Yamaguchi, K. Sato
- 1098.** Influence of the volume and rigidity of ancillary ligand in cyclometalated Ir(III) complexes with applications in Light Emitting Electrochemical Cells (LECs).
P. Dreyse*, I. González, D. Cortés-Arrigada, O. Ramirez, I. Salas
- 1099.** Luminescence of Tris(oxyalato)chromate(III), Tris(malonato)chromate(III) and Tris(2,2'-bipyridine)ruthenium(II) complexes in frozen mixed-solvent of water and ethanol.
T. Otsuka*, Y. Kaizu, A. Inagawa, T. Okada
- 1100.** Synthesis and photophysical properties of poly(pyrlyl) ruthenium(II) complexes having stable radical substituents.
A. Ito, N. Kobayashi, Y. Teki
- 1101.** Development of phthalocyanine-based fluorescence probes for detecting ascorbic acid.
T. Yoko, K. Ishii*
- 1102.** Effect of cavity size toward photochemical properties of a ruthenium(II) terpyridyl group encapsulated in cage-type ligands.
K. Hara*, T. Hatanaka, Y. Furunashi
- 1103.** Synthesis and luminescence properties of ionic liquid based on an anionic cyclometalated Pt(II) complex.
T. Ogawa, M. Yoshida, A. Kobayashi, M. Kato
- 1104.** Magneto-optical effects of phthalocyanine-based thin films on ferromagnetic inorganic substrates.
M. Karasawa, K. Ishii*
- 1105.** Near-infrared Os(II) phosphors with metal-ligand-to-ligand charge transfer transition character.
Y. Chi, J. Liao
- 1106.** Reversible spectral change of copper(II) complexes bearing a 2-(2'-pyridyl)-benzimidazole ligand.
T. Miura, M. Nishikawa, T. Tsubomura*
- 1107.** Development of near-infrared-light induced electron transfer system based on distorted phthalocyanine.
E. Takafumi, M. Kondo, S. Masaoka
- 1108.** Photoisomerization of bis-cyclometalated iridium(III) complexes with a tertiary phosphite ancillary ligand.
H. Konno*, Y. Ido, K. Koike
- 1109.** Development of a novel measurement system for magneto-chiral dichroism using a pulsed electromagnet.
S. Hattori, T. Miyatake, K. Ishii*
- 1110.** Molecular catalysis in photochemical hydrogen evolution from water driven with low driving forces.
K. Yamauchi, K. Kawano, K. Koshiba, K. Sakai*
- 1111.** Design of ratiometric fluorescent probes based on arene-metal ion contact and their application to imaging of hydrogen sulfide in living cells.
R. Kawagoe, I. Takashima, A. Ojida
- 1112.** Synthesis and luminescence of sterically regulated iridium complexes.
Y. Koga, K. Matsubara
- 1113.** Emission-color tuning of stable Cu(I) complexes based on systematic introduction of aromatic rings to diphosphine ligands.
Y. Okano, H. Ohara, M. Yoshida, A. Kobayashi, M. Kato

Hawaii Convention Center
Halls I, II, III

Novel Heme Proteins and Model Systems (#305)

Organized by: J. Dawson, T. Hayashi,
M. Stillman
Presiding: J. Dawson, T. Hayashi,
M. Stillman

Poster Session

19:00 – 21:00

1114. Hemoglobin-albumin clusters having different mammalian hemoglobin as an O₂-binding site.
K. Yokomaku, R. Shinohara, T. Komatsu*

1115. Human(hemoglobin-albumin) clusters having various O₂-affinities.
R. Shinohara, T. Komatsu*

1116. Using free radical metabolites to distinguish the similarities and differences of haem and non-heme peroxidases.
S. Khan*, N. Aljuhani*, K. Michail,
A. Morgan, **A. Siraki**

1117. Iron porphyrin carbene catalytic intermediates: Ferrous or ferryl?. R. Khade, W. Fan, Y. Ling, L. Yang, **Y. Zhang**

1118. Modification of small heme proteins to produce novel organometallic catalysts that function in water.
M.W. Wolf

1119. Metalloprotein design using genetic code expansion.
J. Wang*

120. Molecular basis of heme transfer between NEAT transporters in *Staphylococcus aureus*.
J.M. Caaveiro, K. Morante, N. Vu, Y. Moriwaki, K. Tsumoto

121. Regulation of electronic structures of iron(II) porphyrin radical cation complexes by means of axial ligands.
A. Ikezaki, M. Takahashi, T. Ikeue, M. Nakamura

122. Myoglobins reconstituted with cobalt tetra- and bis-dehydrocorrin as a methionine synthase model.
Y. Morita, K. Oohora, T. Hayashi

123. Isd cog-wheel kinetics. Heme shuttle pathway in *Staphylococcus aureus*.
M. Stillman*

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Metal Coordination Sphere Design for Challenging Bond Transformations (#318)

Organized by: K. Caulton, A. Hill,
S. Johnson, M. Yamashita
Presiding: P.J. Brothers, S.N. Brown,
M. Yamashita

19:00 – 1124. Novel C-E activations induced by pincer type ligands.
R.D. Young*

19:15 – 1125. Synthesis and reactions of multiproton-responsive complexes bearing poly(pyrazole)-type ligands.
S. Kuwata*

19:30 – 1126. Complexes with appended functionality to regulate reductive catalysis.
N. Szymczak, C. Moore, J. Géry,
K. Tseng

19:45 – 1127. General routes to terminal and bridged complexes of carbynes, physical properties of carbide as a ligand.
A. Reinholdt, T.J. Morsing,
J.E. Vibenholt, M. Schau-Magnussen,
K. Herbst, J. Bendix

20:00 – 1128. Cooperative small molecule activation at the nickel-carbon double bond of nickel PC₂carbeneP pincer complexes.
E.A. LaPierre, W.E. Piers*,
D. Spasuk

20:15 – 1129. Catalytic dehydrocoupling of amine-boranes.
E. Leitao, I. Manners

20:30 – 1130. Versatile reactivity of borylene complexes: Metathesis, borylene-carbonyl coupling and more.
H. Braunschweig, **R. Shang**

20:45 – 1131. High-spin clusters: Creating reaction sites for small molecule activation.
T. Betley

Friday Morning

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson, G. Schreckenbach, T. Yaita, J. Li,
P. Yang
Presiding: J. Gibson, P. YANG

8:00 Introductory Remarks

8:05 – 1132. Theoretical studies of orbital mixing in actinide-ligand bond.
E.R. Batista*

8:35 – 1133. Soft X-ray synchrotron radiation spectroscopy of radioactive materials coupled with theory: Increasing the impact.
D.K. Shuh*

9:05 – 1134. Molecular design of *N,N*-dialkyl monoamide for selective separation of U(VI).
S. Suzuki*, T. Kobayashi, H. Shiwaku, T. Yaita

9:35 – 1135. Size recognition properties of multidentate N-donor ligands for f-series elements.
M. Nakase*, T. Kobayashi, K. Takeshita, H. Shiwaku, T. Yaita

9:55 Break

10:10 – 1136. Chemical periodicity and the chemistry of protactinium.
R. Wilson*, V. Vallet

10:40 – 1137. Calculating magnetic properties of actinide complexes from first principles.
J. Autschbach

11:10 – 1138. Thermochemistry of gas-phase actinide molecular ions.
P.B. Armentrout

11:40 – 1139. Computational studies of actinide "Pacman" complexes.
G. Schreckenbach*, Q. Pan, X. Zhang

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Functional Nanomaterials Based on Coordination Chemistry (#73)

Organized by: T. Uemura,
M. MacLachlan, H. Matsui
Presiding: H. Matsui

8:00 – 1140. Exploiting the confined environment of P22 virus-like particles for chemical catalysis.
T. Douglas

8:25 – 1141. Viruses as building blocks for functional nanomaterials development.
Q. Wang

8:45 – 1142. Versatile nanoscale Prussian blue coordination polymers: Design, preparation, characterization, and multimodal biomedical imaging of Prussian blue analogs.
K. Sorasaenee*, P. Promdet, B. Rodriguez, A. Henry, T. Khuu, A. Hovsepian, J. Galan-Mascaros

9:00 – 1143. Short peptides self-assemble in the presence of metals to produce catalytic nanomaterials. C. Rufo, Y. Moroz, O. Moroz, O. Makhluyets, P. Gosavi, J. Stoehr, T. Smith, X. Hu, W. DeGrado, I. Korendovich

9:15 – 1144. Designing protein crystals for bioinorganic nanomaterials.
T. Ueno*

9:35 – 1145. Exploiting the specific, non-covalent, interactions of peptides with inorganic nanoparticles to engineer functional and responsive interfaces on the atomic scale.
M.R. Knecht

9:55 break

10:05 – 1146. Selective uranyl binding by a protein-based reagent.
C. He*

10:25 – 1147. Programmable metal array arrangement on peptides: Composition- and configuration-controlled heterometallic hybrid materials.
H.R. Takaya*

10:45 – 1148. Manipulating the interface between biomolecules and nanomaterials: Challenges and advances for bridging theory and experiment.
T.R. Walsh*, L. Wright, J. Palaofox-Hernandez, Z.E. Hughes, K.L. Drew

11:05 – 1149. Utilizing nascent protein interaction sites to construct hybrid natural/synthetic nanostructures.
V. Nanda

11:25 – 1150. Stimuli-responsive pi-conjugated systems bearing rotational units.
M. Takeuchi, **A. Takai**

11:45 – 1151. Liquid crystalline metallomacrocycles toward soft materials with nanospaces.
S. Kawano, K. Tanaka*

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Recent Discoveries in the Chemistry of Bismuth and Related Elements: the Green Alternative (#93)

Organized by: K. Whitmire, H. Sun,
P. Andrews
Presiding: P. Andrews

8:00 – 1152. Integrative biology approach for investigation of bismuth antiulcer drugs.
H. Sun*, Y. Hong, G. Chan, L. Hu

8:30 – 1153. Recruiting bismuth in the fight against multi-resistant bacteria.
P. Andrews

9:00 – 1154. From bismuth oxido clusters to metal oxide-based materials.
M. Mehring*

9:30 – 1155. Toward understanding and controlling the assembly of bismuth salicylate nanoclusters in solution.
T. Friscic, D. Tan, S.A. Kimber

10:00 Break

10:15 – 1156. Inhibition of urease through disruption of GTPase UreG by bismuth.
H. Li, X. Yang, Y. Chang, H. Sun*

10:30 – 1157. Diversifying the coordination chemistry of bismuth.
N. Burford

11:00 – 1158. Low coordinate bismuth amides: Cations and radicals.
M.P. Coles*, R.J. Schwamm, B.M. Day, J. Harmer, M. Lein, C.M. Fitchett

11:30 – 1159. Novel bismuth-transition metal interactions.
C. Limberg*, C. Tscherisch, C. Herwig, B. Braun

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Coordination and Supramolecular Chemistry for Aqueous Metal Ion Separations (#97)

Organized by: R. Ellis, D. Robinson, R. Motokawa

8:00 – 1160. High throughput method to determine selectivity of ion phase transfer in multi-component chemical systems: Toward predictive modeling of extraction.
H. Moehwald

8:25 – 1161. Design and synthesis of polymer-supported complexants applied to wet process phosphoric acid.
S.D. Alexandratos*, X. Zhu

8:50 – 1162. Microfluidic solvent extraction of rare earth elements.
F.H. Kriel, R.P. Catthoor, S. Middlemas, G. Hatch, C. Priest*

9:15 – 1163. Creation of novel thermo responsive polymer brushes for mutual separation of actinides and lanthanides.
N. Yokachukuse*, K. Park, T. Tsukahara

9:40 – 1164. Extraction and throughput for micro-solvent extraction of platinum using a single chip and a multi-chip module.
F.H. Kriel*, C. Priest, J. Ralston, L. Parkinson, S. Woollam, N. Plint, R.A. Grant, P. Ash

10:05 Break

* Principle Author

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<http://pacificchem.org/onlineprogram>

10:20 – 1165. Relating experimentally measured quantum yields of luminescent lanthanides to their hydration number at different temperatures. A.T. Johnson, A.M. Mattson, M.R. Finck, **L.R. Martin**

10:45 – 1166. Solvation structures of metal ions in a protic ionic liquid (PIL) comprising *N*-alkylethylenediamine and a reversible extraction of transition-metal ions from aqueous media using the PIL. **M. Iida***

11:10 – 1167. Solution and solid-state structural chemistry of tetravalent f-element-organic ligand based compounds. **K.E. Knope**

11:35 – 1168. Metal separation property of macrocyclic and pseudomacrocyclic compounds as extraction reagents. **K. Ohto***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

Frontiers of Molecular Magnetism (#109)

Organized by: H. Oshio, J. Miller, R. Oakley, S. Brooker, S. Gao, M. Ohba
Presiding: M. Ohba, V. Ovcharenko

8:00 – 1169. Stimuli-responsive magnetic molecular materials. **E. Coronado**, G. Abellán, N. Calvo Galve, M. Giménez-Marqués, G. Mínguez Espallargas

8:30 – 1170. Functionalisation of dithiadiazolyl radicals: Toward multifunctional materials. Y. Beldjoudi, **J.M. Rawson**

8:50 – 1171. Valence tautomerism in polynuclear and polymeric complexes. **C. Boskovic***, K. Alley, O. Drath, K. Murray, G. Poneti, L. Sorace

9:10 – 1172. Guest-responsive magnets based on tetracyanometallate building units. **M. Ohba***

9:30 – 1173. Spin transitions in coordination polymer heterostructures. **D.R. Talham***

9:50 Break

10:05 – 1174. Tuning the spin crossover switching temperature by up to 100 K: The importance of pressure, solvent or ‘tail’. **S. Brooker***, H. Feltham, R. Miller, R. Hogue, A. Elliott, K. Gordon, G.B. Jameson, S. Clark, S. Narayanaswamy, J. Tallon

10:25 – 1175. Guest dependent spin transition behavior of Fe(II) and Co(II) coordination polymers. **R. Ohtani**, M. Ohba, S. Kitagawa, S. Hayami

10:45 – 1176. New member of inorganic zeolite family, lanthanide-based sodalite-type zeolite of $[Ln_3(OH)_6CO_3HCOO]_3H_2O$ ($Ln = Gd, Dy, Tb$). Y. Yang, **L. Long**

11:05 – 1177. Supramolecular assembly for the design of molecular magnets. **H. Miyasaka***

11:25 – 1178. Breathing crystals. **V. Ovcharenko***

Hilton Hawaiian Village
Rainbow Tower, Rainbow 1

Electron Transfer and Electrochemistry of Inorganic and Organometallic Materials (#126)

Organized by: H. Nishihara, P. Harvey, W. Wong
Presiding: I. Manners, W. Wong

8:00 – 1179. Manipulating the functional properties of organometallic molecules with hydrocarbyl ligands containing main group moieties. **W. Wong***

8:30 – 1180. Influence of substituents in non-polyicyclic silole-based derivatives on their AIE properties and applications. **B. Tang*, Y. Cai**

9:00 – 1181. Functional metallophosphors for high performance white organic light-emitting diodes. **C. Ho**

9:30 – 1182. Luminescent platinum complexes with long-lived excited states: Photophysical properties, photo-catalysis, and materials application. **C. Che***

10:00 – 1183. Electrochemical and spectroelectrochemical methods to address magnetic and optical switching in electroactive molecular materials. **B. Sarkar**

10:20 – 1184. Photoelectrochemical performance of corrosion layer formed on weathering steel surface. **P. Qiu***, L. LUO, C. Chen

10:40 – 1185. Functional metallocopolymers based on metallocenes of iron, cobalt, and nickel. **I. Manners***

11:10 – 1186. Electronic interactions in boron-containing organometallic oligomers and polymers. **F. Jaekle***

11:40 – 1187. Crystal structures and carrier transport properties of mixed-valence coordination polymers with dithiocarbamate derivatives. **T. Okubo***, K. Tanishima, Y. Kono, K. Himoto, K. Nakatani, M. Maekawa, T. Kuroda-Sowa

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170)

Organized by: K. Theopold, K. Mashima, Z. Xie
Presiding: Z. Xie

8:00 – 1188. Chelating σ -aryl and related post-metallocenes: Unusual reaction pathways and intramolecular interactions. **M. Chan**

8:30 – 1189. Electrocatalytic activation of CO_2 by a series of rhodium complexes. **K. Mullick***, A. Angeles-Bоза

8:50 – 1190. Generation and reactivity of low-valent Group 5 imido complexes. **J. Arnold***

9:20 – 1191. Zr(IV) cations: Small molecule activation and catalytic imine hydrogenation. **O. Metters**, S.R. Flynn, D. Wass*, I. Manners*

9:40 – 1192. Catalytic radical addition and hydrodehalogenation reactions by niobium and tantalum complexes bearing 1,4-diaza-1,3-butadiene ligand. **H. Nishiyama**, T. Saito, H. Tsurugi, K. Mashima

10:00 – 1193. Tl^{II}/Tl^{IV} redox catalysis: [2+2+1] synthesis of pyrroles from alkynes and diazenes. **I.A. Tonks***

10:20 – 1194. Rare-earth metal alkylidene and imide complexes. **R. Anwander***, D. Schäde, L.N. Jende, A. Krenzer, C. Maičiūtė-Mössmer, C. Schäde, K.W. Törmroos

10:50 – 1195. Dimerization of acene derivatives. **Z. Song**, S. Zhang, K. Nakajima, T. Takahashi*

11:10 – 1196. Low-valent titanium catalyzed deprotection of alloc- and poc-amides. **S.M. Vasanthakumari**, H. Takagi, C. Matsuno, S. Okamoto*

11:30 – 1197. Salt-free reduction of early transition metal complexes by 1,4-bis(trimethylsilyl)-1,4-diaza-2,5-cyclohexadienes for activating small molecules. **K. Mashima***, T. Saito, H. Nishiyama, K. Kawakita, H. Tanahashi, H. Tsurugi

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

Transition Metal Complexes of N-Heterocyclic and Mesoinionic Carbenes: Structure, Materials and Catalytic Applications. (#195)

Organized by: C. Crudden, S. Chang, M. Albrecht, D. Allen, U. Complete

8:00 – 1198. Macrocyclic N-heterocyclic tetra-carbene complexes that perform innovative catalytic aziridinations. **P.P. Chandrapud, C.L. Keller, D.M. Jenkins**

8:20 – 1199. Paradoxical effects of strong NHC donation in catalysis. **D. Fogg**

8:50 – 1200. Simple synthesis of metal complexes of *N*-heterocyclic carbenes and their catalytic applications. **W. Chen**

9:10 – 1201. Polyaromatic N-heterocyclic carbenes and π -stacking: Catalytic consequences. **E. Peris***

9:40 – 1202. Copolymerization of olefins and polar monomers by Pd/IzQO catalysts. **R. Nakano**, K. Nozaki

10:00 – 1203. New heterocyclic carbene ligand that contains transition metal π -donor substituents. **S. Takemoto***

10:20 – 1204. Reactive metal–element and metal–metal bonds in group 11 metal complexes. **J.P. Sadighi***, C.M. Wyss, B.K. Tate, T.J. Robilotto, N.T. Daugherty, J. Bacsa

10:50 – 1205. NHC-copper-catalyzed carboxylation reactions using carbon dioxide as a building block. **Z. Hou***

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239)

Organized by: K. Ishii, Z. Chen, P. Ford, G. Hanan

8:00 – 1206. Photobiological and theranostic aspects of ruthenium compounds as modulators of nitric oxide and singlet oxygen by light irradiation: The synergistic effect. **R.S. da Silva***, L. Ramos, J. Uzelli

8:25 – 1207. Modular ruthenium complexes containing both DNA groove binding and intercalative units. **M.G. Walker**, J. Thomas

8:40 – 1208. Photoactivated precious metal anticancer and antibacterial complexes. **P.J. Sadler***

9:05 – 1209. Design and synthesis of C_3 -symmetric and luminescent tris-cyclometalated iridium(III) complexes having biologically active peptides. **Y. Hisamatsu***, A. Shibuya, N. Suzuki, H. Tanaka, A. Masum, S. Aoki

9:20 – 1210. Transition metal complexes for phototherapy. **C. Turro**, K. Dunbar

9:45 – 1211. Controlled release of carbon monoxide from photoactive metal-organic framework. **A. Carne-Sánchez**, J. Zhang, C. Kim, S. Diring, S. Furukawa*, S. Kitagawa*

10:00 Coffee break

10:10 – 1212. NO and CO releasing materials. **A. Schiller***

10:30 – 1213. Strategies for the photochemical uncaging of bioactive small molecules. **P.C. Ford***

10:55 – 1214. Photophysics and reverse saturable absorption of Pt(II) bipyrlyl bis-acetylidyne complexes with extended π -conjugation. **W. Sun***, R. Liu, Y. Li, T. Lu

11:10 – 1215. Highly luminescent imidoylamidinato platinum(II) complexes formed by the coupling of 1*H*-pyrazole-1-carboxamide with nitriles used as reaction solvents. **K. Umakoshi***, R. Nouchi, T. Tanaka, Y. Nakao, Y. Arikawa

11:25 – 1216. Recent advances in developing highly efficient phosphorescent platinum complexes. **S. Huo***

11:40 – 1217. Theoretical studies of thermal deactivation processes of phosphorescent states in Pt(II) complexes. **K. Nozaki***, J. Maeba, M. Iwamura

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2

Inorganic Complexes for Solar Energy Harvesting (#256)

Organized by: M. Wolf, K. Sakai, F. MacDonnell
Presiding: M.O. Wolf

8:00 – 1218. Ruthenium polypyridyl complexes that photo-oxidize halide ions in fluid solution and at TiO₂ interfaces. **G. Li**, E. Beauvilliers, W. Swords, **g. meyer***

8:35 – 1219. Group 8 transition-metal azolate complexes for dye-sensitized solar cells. **Y. Chi**

9:10 – 1220. Trapped in imidazole: How to accumulate multiple photoelectrons on a black absorbing ruthenium complex. **B. Dietzel**

9:30 – 1221. Interfacial dynamics in the dye-sensitized solar cell. **C.P. Berlinguet***

10:05 Break

10:20 – 1222. Novel redox mediators for dye-sensitized solar cells. **U. Bach**

10:55 – 1223. Photohydrides for tightly integrating visible light absorption with hydride transfer. **A. Miller***, C. Pitman, S. Barrett, K. Brereton

11:15 – 1224. Driving proton-coupled electron transfer reactions with solar photons. **J.L. Dempsey***, T.T. Eisenhart, D.A. Kurtz, J.C. Lennox

11:35 – 1225. Photo-driven charge storage coupled with catalytic water reduction to hydrogen. **K. Sakai**

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

Metal Mediated Polymerization (#292)

Organized by: P. Hayes, R. Waterman, T. Mizuta, Y. Tang, P. Sangstrutnugul
Presiding: F. Kerton, M. Shaver

8:00 – 1226. Selective bond formation between hetero atoms catalyzed by a transition metal complex. **H. Nakazawa***

8:30 – 1227. Synthesis of functional and topological polyesters mediated by metal coordination catalysts. **W. Zhao**, Y. Wang, **D. Cui***

9:00 – 1228. New iron complexes for atom transfer radical polymerization and organometallic mediated radical polymerization. **M. Shaver***

9:30 Intermission

9:40 – 1229. Metal-based reactions for phosphorus-containing polymeric materials. **R. Waterman**

10:10 – 1230. Catalytic precision polymerization: From polar monomers to functional materials. **A. Kronast**, B. Rieger

10:30 – 1231. Rhodium mediated carbene insertion polymerization: Mechanism and stereoregulation. **B. de Bruin***

11:00 – 1232. Metal-mediated catalytic ring-opening of macrolactones to polyethylene-like polyesters. **R. Duchateau**, L. Jasinska, M. Bouyahyi, M. Pepels

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Novel Heme Proteins and Model Systems (#305)

Organized by: J. Dawson, T. Hayashi, M. Stillman
Presiding: T. Hayashi

8:00 break

8:40 – 1233. On the O-O bond cleavage processes of endoperoxide and alkyl hydroperoxide mediated by iron porphyrin coordinated by thiolate. **T. Higuchi***

9:00 – 1234. Mechanism of effective nitric oxide decomposition in microbial denitrification. **T. Tosa***, E. Teraska, K. Matsumoto, H. Sugimoto, Y. Shiro

9:20 – 1235. Heme oxygenase catalytic mechanism. **M. Ikeda-Saito**, T. Matsui, M. Unno

9:40 – 1236. Ligand switching and redox reactions in engineered heme proteins. **E. Pletnev***

10:00 – 1237. Osmotic pressure effects reveal a specific dehydration-induced hydrophobic electron transfer structure comprising cytochrome c and cytochrome c oxidase. **K. Ishimori***

* Principle Author

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- 10:20 – 1238.** Factors controlling access to alternate conformers of mitochondrial cytochrome c. **B.E. Bowler***, L.J. McClelland, E.M. Nold, S. Bandi, S.R. Sprang, T. Mou
- 10:40 – 1239.** Metalloprotein design using genetic code expansion. **X. Liu***, J. Wang*
- 11:00 – 1240.** Engineering solid-state heme proteins. **T.D. Rapson***, T. Sutherland, J.S. Church, A.C. Warden, J. Liu, H.E. Trueman, H. Dacres, S.C. Trowell
- 11:20 – 1241.** Visible light induced carbon dioxide conversion with the system consisting of water soluble metalloporphyrin and dehydrogenase. **Y. Amao***
- 11:40 – 1242.** Construction of heme protein oligomers by domain swapping. **S. Hirota***

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Metal Coordination Sphere Design for Challenging Bond Transformations (#318)

Organized by: K. Caulton, A. Hill,
S. Johnson, M. Yamashita
Presiding: A.F. Hill, W.E. Piers, A.S. Veige

- 8:00 – 1243.** Modular ligand designs for small molecule activation. **M. Fryzuk**, S. Westhues, T.G. Ostapowicz, V.T. Annibale, T.C. Wambach, C. Lenczyk
- 8:20 – 1244.** Catalysis of dehydrogenative borylation of terminal alkynes. **O.V. Ozerov**, C. Lee, J. Zhou, J. DeMott, W. Shih, N. Bhuvanesh

- 8:40 – 1245.** Ligand design in organometallic chemistry taken to the extreme: When the metal is no longer needed. **F. Fontaine***, M. Courtemanche, M. Legare, E. Rochette
- 9:00 – 1246.** New types of olefin metathesis ruthenium catalysts featuring fluorinated N-heterocyclic carbenes and chelating indenylidene ligands. **C. Bruneau***, S.N. Osipov, S. Masoud, C. Fischmeister, P.H. Dixneuf

- 9:15 – 1247.** Ligand design for nonclassical oxygen atom transfer reactions. **S.N. Brown***
- 9:30 – 1248.** Selective reduction of carbon dioxide to bis(silylacetals) mediated by a PBP-supported nickel complex. P. Ríos, J. López-Serrano, **M.A. Rodriguez***

- 9:45 – 1249.** Managing productive reactivity and competitive deactivation with cooperative ligands. **J.M. Blacquière***
- 10:00 – 1250.** Synthesis, structures and reactivity of metallacarbaranes. W. Sattler, S. Ruccolo, **G. Parkin***

- 10:20 – 1251.** Ambiphilic ligand design for the development of cooperative reactivity. **D. Emslie***, B. Cowie
- 10:40 – 1252.** Reactivity of a new class of monoanionic nitrogen donor. **S.A. Johnson***, V. Semeniuchenko, S. Zhu

- 11:00 – 1253.** Polynuclear complexes consisting of ambidentate ligands. **F. Breher***
- 11:15 – 1254.** Rh-complexes in homogeneous catalysis - activation and deactivation phenomena. **D. Heller***, H. Drexl, A. Meissner, E. Alberico, A. Koenig

- 11:30 – 1255.** Tuning the chemistry of boron - macrocyclic polypyrrrole ligands. S. Maslek, A. Tay, N. Novikova, M.C. Simpson, **P.J. Brothers***
- 11:45 Flash 3**

Hawaii Convention Center
Halls I, II, III

Telomeres and other G-quadruplex Structures as Targets for Metallodrugs (#459)

Organized by: J. Aldrich-Wright, N. Sugimoto, J. Chaires, S. Ralph

Poster Session
10:00 – 12:00

- 1256.** Probing metal complex/quadruplex DNA interactions using mass spectrometry and cd spectroscopy. **S.F. Ralph***, N. Assadawi, K. Davis

- 1257.** Chiral dinuclear ruthenium (II) complexes as two-photon, time-resolved emission microscopy probes for duplex and quadruplex DNA. **C.L. Glover***, J. Thomas, N. Green
- 1258.** Drug-induced stabilization of the hTERT G-quadruplex results in reversal of mutant promoter activation. **H. Kang**, H. Mao, L.H. Hurley*
- 1259.** Monitoring of extracellular potassium ion based on G-rich oligonucleotides. N. Sakamoto, S. Sato, **S. Takenaka**
- 1260.** Binding interactions of ruthenium-based prodrugs with tRNA. B. Dwyer, R. Josephson, E. Johnson, S. Kirk, **K.M. Holman***
- 1261.** Probing G-quadruplex structures: TWIMS investigations of a bimolecular G-quadruplex and duplex DNA/RNA hybrid. **M.L. Birrento***, S. Samosorn, T.M. Bryan, J.L. Beck
- 1262.** NMR study of chiral dinuclear Ruthenium complexes and their interaction with DNA motifs. **s.d. fairbanks**, M. Williamson, J. Thomas
- 1263.** Ellipticine analogs as PDGFR G-quadruplex interactive agents for the treatment of cancer and acute lung injury (ALI). R. Brown, H. Quijada, S. Camp, E. Chiang, **V. Gokhale**, T. Wang, J. Garcia, L.H. Hurley*
- 1264.** Telomerase inhibitor assay by using electrochemical method based on chronocoulometric technique. **S. Sato**, S. Takenaka
- Hawaii Convention Center
Halls I, II, III
- Inorganic General Posters**
10:00 – 12:00
- Catalysis**
- 1265.** Reduction of pyridine derivatives using E-B reagents (E=P,B), **S.J. Geier**, C.M. Vogels, A. Decken, S. Doherty, S. Westcott*
- 1266.** Effect of the A-site on ammonia synthesis with perovskite oxyhydride-supported Ru catalysts. **Y. Tang**, **Y. Kobayashi**, N. Masuda, **S. Hosokawa**, C. Tassel, **T. Yamamoto**, **H. Kageyama**
- 1267.** Iron-amine-phenolate complexes as catalysts for bond-forming reactions. **E.D. Butler**, C.M. Koza
- 1268.** Ferrocenyl phosphonium cations as synthetically facile Lewis acids in organocatalysis. **I. Malloy***, D. Stephan
- 1269.** Catalytic reduction of phosphine oxides to phosphines by electrophilic phosphonium cations (EPCs). **M. Mehta***, I. Garcia, M. Perez, D. Stephan
- 1270.** Counterion effect in gold catalyzed dearomatization of indoles with allen-amides. L. Rocchigiani, M. Jia, M. Bandini, **A. Macchioni**
- 1271.** Hybrid NH ligands: Versatile platforms for multinuclear complexes with improved catalytic activities. **D. Mendoza-Espinosa***, G. Negron-Silva
- 1272.** New siloxane coupling reaction with Lewis acid catalyst. **K. Hayashi**, N. Terashita, R. Nakajima, N. Takeda, M. Unno
- 1273.** Iron-catalyzed reductive magnesiation of octanes and metallocyclic cyclization of alkynyl octanes. **Y. Tanabe**, Y. Sugiyama, S. Heigozono, K. Tamura, S. Okamoto*
- 1274.** Cationic metallogermylene and a cationic germlylene complex: Syntheses and reactivity toward H₂. **K. Inomata**, T. Watanabe, H. Hobita*
- Materials with unique electronic or optical properties**
- 1275.** Synthesis of bis(dipyririnato)zinc(II) complexes fluorescing brightly in longer wavelength region. **T. Iwashima**, M. Tsuchiya, S. Kusaka, R. Sakamoto*, H. Nishihara*
- 1276.** Graphene-encapsulated NiO-NiFe₂O₄ nanocomposites as anode materials for Li-ion batteries. **D. Du**
- 1277.** Synthesis, electrochemistry and single-molecule conductance of bi-metallic 2,3,5,6-tetra(pyridine-2-yl)pyrazine based complexes. **R. Davidson***
- 1278.** Second-harmonic generation (SHG) and photoluminescence (PL) properties of Diòn-Jacobson type polar layered perovskites solid-solutions, CsBi_{1-x}Eu_xNb₂O₇ (x = 0, 0.1, and 0.2). **H. Kim***
- 1279.** Graphene oxide and reduced graphene oxide hybrids with spin crossover iron(III) complexes. **Y. Murashima***, H. Takehira, K. Wakata, R. Ohtani, m. nakamura, S. Hayami
- 1280.** High proton conductivity of graphene oxide hybrids. **K. Wakata***, Y. Murashima, H. Takehira, R. Ohtani, m. nakamura, S. Hayami
- 1281.** Ligand exchange between amines and metal-carboxylates on metal-chalcogenide nanocrystals. **Y. Zhou**, F. Wang, y. wang, W.E. Buhro
- 1282.** Greenish-blue phosphorescent iridium(III) complexes with hexylcarbazole-substituted carbene derivatives for organic light-emitting diodes (OLEDs). **Y. Kim***, Y. Song, W. Cho, S. Jin
- 1283.** Syntheses of cyclometalated square-planar platinum(II) complexes with boronic acid ligands and their reactivities toward D-fructose. **K. Fukuda**, T. Sugaya, K. Ishihara*
- Magnetic Materials**
- 1284.** Structure and magnetic property of cobalt(II) compounds with adenine and thymine substituents. **M. Nakaya**, H. Ohmagari, R. Ohtani, m. nakamura, S. Hayami
- 1285.** Magnetic behaviors of Iron(II) and Iron(III) complexes incorporating the same Schiff base ligand. **N. Saigo***, K. Hirata, R. Ohtani, m. nakamura, S. Hayami
- 1286.** Excimer formations of Co(II) spin-crossover complexes with π conjugated ligands. **R. Nakahara***, S. Egawa, M. Nakaya, R. Ohtani, m. nakamura, S. Hayami
- 1287.** Magnetic interaction of mononuclear metal complexes with helical structure. **H. Ohmagari***, M. Nakaya, R. Ohtani, m. nakamura, S. Hayami
- 1288.** Spin frustration of mixed spin system, $\text{Co}_{1-x}\text{Ti}_x\text{S}_2$. **K. Hayashi***
- 1289.** Magnetic behaviors and oxidation reactions of cobalt(II) complexes with strand-type hexadentate ligands containing thioether and amide donor groups. **T. Tada***, Y. Yamane, Y. Sunatsuki, T. Suzuki, M. Kojima
- 1290.** Magnetic behavior and liquid crystal properties of iron(II) complexes with long alkylated bzimpy ligands. **Y. Sekimoto***, R. Ohtani, m. nakamura, S. Hayami
- 1291.** Magneto-electric control of multiferroic domains in $\text{A}_2\text{MS}_2\text{O}_7$ ($\text{A} = (\text{Sr}, \text{Eu})$, $\text{M} = (\text{Co}, \text{Mn})$) crystals. **K. Nishina***, R. Kajihara, R. Oda, M. Akaki, H. Kuroe, K. Itatani, H. Kuwahara
- Cluster Chemistry**
- 1292.** Controllable regioselective activation of $\mu_2\text{-O}$ in Anderson cluster towards single-side triol-functionalized χ isomers synthesis and proton-controlled isomerization transformation. **Z. Zhang**, Y. Wei
- 1293.** Multinuclear iron(II) complexes bridged by bis-bidentate type Schiff base ligands containing two imidazole groups. **T. Tanaka**, T. Suzuki, Y. Sunatsuki
- 1294.** Synthesis of new Fe₄₂ cyanide-bridged nanocages: Toward control of electronic structures. **S. Nishino***, S. Kang, S. Kanegawa, O. Sato
- Inorganic Materials**
- 1295.** Preparation of zinc oxide thin film by atmospheric pressure chemical vapor deposition. **H. Hayakawa***, Y. Akiyama
- 1296.** Cation-controlled interlocked coordination polymers and solvent-triggered supramolecular isomers exhibiting reversible SCSC transformation. **H. Ju***, M. Ikeda, Y. Habata, S. Lee
- 1297.** Crystal engineering of endo/exocyclic coordination polymers with rationally designed ditopic macrocycles and guest-exchanges in crystalline state. **E. Lee***, K. Park, M. Ikeda, S. Kuwahara, Y. Habata, S. Lee
- 1298.** Palladium(II) mononuclear and palladium(II)/ruthenium(II) heterodinuclear complexes bearing a quinoline-2-carbaldehyde (pyridine-2-carbonyl)hydrazone. **Y. Nakatani***, A. Mori, T. Suzuki, Y. Sunatsuki, K. Nakajima
- 1299.** Hydrogen bond induced photoluminescence behavior of iridium(III) complexes. **T. Sugaya***, F. Takahashi, S. Takata, K. Isoda, M. Tadokoro, K. Ishihara
- 1300.** Photofunctional 1D coordination polymers based on bis(dipyririnato)zinc(II) complex. **R. Toyoda**, R. Matsuoka, M. Tsuchiya, R. Sakamoto*, H. Nishihara*
- 1301.** Rapid approach to find product separations using a coupled GC-ICP-TOF-MS system. **S.A. Stratz***, J. Auxier, A. Jones, H. Hall
- Co-ordination Chemistry**
- 1302.** Coordination variability of Cu^I in multidentate heterocyclic thioamides: Synthesis, crystal structures, luminescent properties, and ESI-mass studies of complexes. **A. Kaur**, T. lobana
- 1303.** Synthesis and kaleidoscopic reactivities of bis(tritylgermyl)bis(dimethylphenylphosphine)platinum(II). **Y. Ogata**, K. Mochida*
- 1304.** Metal chelating properties of 6-imino-2-(1,2,3-triazol-4-yl)pyridines. M. Dillenburg, **J. Fletcher**
- 1305.** Synthesis, Lewis adducts, and electrochemical as well as optical properties of two pnicogen-containing trigonal-planar complexes $[\text{E}(\text{Cr}(\text{CO})_3)_3]$ ($\text{E} = \text{Sb}, \text{Bi}$). **C. Yu**, K. Hsing, Z. Sun, M. Shieh*
- 1306.** Synthesis and properties of $\text{Cp}^*\text{W}(\text{NO})(\text{H})\langle\gamma^3\text{-allyl}\rangle$: A new family of tungsten nitrosyl complexes. **M.V. Shree**, P. Legzdins*, R.A. Bailie, R.J. Wakeham, A.S. Holmes, G.P. Lefèvre
- 1307.** Synthesis, structures, and properties of mono-, di-, and tetranuclear manganese complexes with unsymmetrical ligands derived from N -(aminoalkyl)salicylamide. **R. Ogawa***, R. Mitsuhashi, T. Suzuki, Y. Sunatsuki, R. Ishikawa, S. Kawata
- 1308.** Influence of the equatorial halide ligands on the axial ligand substitution reactions of pivalamido-bridged Pt(IV) binuclear complexes with halide ions and olefins. **Y. Kamezaki**, T. Terada, J. Toda, T. Sugaya, S. Iwatsuki, K. Ishihara*, K. Matsumoto
- 1309.** Influence of terminal ligands on the electronic density of $[\text{Ru}_3\text{O}(\text{CH}_3\text{COO})_6(\text{CO})_2\text{L}]$ complexes ($\text{L} = \text{N-heterocyclic ligands}$). **M.B. Moreira***, S. Nikolau
- 1310.** Exploration of new anionic selenium based pincer ligands. **B.J. Charette***, J.S. Ritch
- 1311.** Multiphase inspection of the conformational variations in formamidines. **M.B. Pastor**, M. Tsai, Q. Zhao*
- 1312.** Insertion of first row transition metal carbonyls into the dimetallyles of germanium and tin. **M.L. McCrea-Hendrick**, P.P. Power
- 1313.** Effective siloxane cleavage reaction. **J. Ueno***, R. Shimada, N. Takeda, M. Unno
- 1314.** Nucleophilic ligands based on boron. **D. Vidovic**

* Principle Author

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1315. Synthesis and characterization of imogolite nanotube functionalized with methyl groups from the precursor solution. **K. Yamamoto***, M. Sugihita
1316. Arene-ruthenium trigonal cage with borane core for sensing cyanide ion. **J. Ryu**, Y. Park, M. Lee*, J. Lee*

Solid state chemistry

1317. Calorimetric study of the oxide-framework conversion reaction of hydrated alkali-metal polybromide bronze at room temperature. **T. Suzuki***, A. Tanaka, T. Nishida, K. Eda
1318. Structural feature of SrGeO₃ high-pressure perovskite phase studied by single-crystal X-ray diffraction. **A. Nakatsuka***, H. Arima, O. Ohtaka, K. Fujiwara, A. Yoshiasa
1319. Cation distribution of Na GTS-type titanosilicates ion-exchanged by Er³⁺. **K. Fujiwara***, K. Shinohara, A. Nakatsuka
1320. Exocyclic coordination networks of O₂S₂-macrocycles: Self-assembly and solvent-induced SCSC transformation. **S. Kim***, L.F. Lindoy, S. Lee
1321. ³¹P and ⁵¹V NMR studies of the di- and triphosphate-(peroxy)vanadate(V) systems. **S. Sorishita***, M. Hashimoto
1322. Enthalpy and heat capacity measurements of high-pressure Fe(II)-silicates and thermodynamic calculation of phase diagrams of Fe₂SiO₄ and FeSiO₃. **T. Kitajima**, H. Kojitani, M. Akaogi*
1323. Variable frameworks and centricities found in a series of quaternary scandium selenites. **S. Song***
1324. Glass transition and crystallization properties study of Ni-Nb-Zr glassy alloys. **A. Uchida**
1325. Preparation of lithium-doped zinc oxide thin film by LPCVD method. **K. Misawa***, Y. Akiyama
1326. Relationship between composition and thermal/electrical properties of sintered zirconium carbide. **S. Yagishita**, K. Ozaki, H. Nakayama, Y. Nakajima, T. Nabeta
1327. Development of a synthetic pathway for polybdenum-phosphorus complexes. **L. Claussen**, R.K. Thomson
1328. Dissolution of aluminum mineral polymorphs to study Al³⁺ oxo-hydroxo clusters in solution. **B.L. Fulton**, D.W. Johnson*, J. Hutchison

Bio-Inorganic

1329. Luminescent metal ion complexes for live cell imaging. **T.A. Gillam***, D. Brooks, M. Massi, S. Plush
1330. Antidiabetic effect of Zn complexes with organochalcogen-containing ligands. **T. Nishiguchi**, Y. Yoshikawa, H. Yasui*
1331. Anticancer activity and reduction kinetics of platinum(IV) metallocointercalators. **K. Deo**, F. Macias, B.J. Pages, P. Wormell, F. Li, J. Aldrich-Wright*

Remediation

1332. Separation of sodium and zinc impurities from diesel fuel based on ionic liquids. **P.J. Corbett**, J.P. Hallett
1333. Preparation of silica gel and its application for removal of heavy metal ions from aqueous solutions. **H. Minamisawa**, H. Asamoto, M. Minamisawa, T. Nakagama

Boron chemistry

1334. Syntheses and properties of iridium(III) complexes bearing diol ligands and their reactivity to boric acid. **Y. Tabel**, Y. Fujioka, T. Sugaya, K. Ishihara*
1335. Syntheses and properties of platinum(IV) complexes having diol moiety and their reactivity to boric acid. **Y. Samukawa**, Y. Gu, T. Sugaya, K. Ishihara*
1336. Kinetic study on the reaction of diphenylborinic acid with D-fructose. **Y. Sobue**, T. Sugaya, S. Iwatsuki, K. Ishihara*
1337. Synthesis and characterization of lithium and mixed alkali metal borates. **B. Yonke**, D. Wilson, D. Neiner, D.M. Schubert

Friday Afternoon

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3
Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson, G. Schreckenbach, T. Yaita, J. Li, P. Yang
Presiding: A.E. Clark, D.K. Shuh

13:00 – 1338. Structural diversity and spectroscopic properties of uranium phosphonates. T. Zheng, L. Chen, **J. Diwu***, Z. Chai, S. Wang*, T.E. Albrecht-Schmitt
13:20 – 1339. Actinide chemistry in the gas phase: A fruitful interplay between experiment and theory. **J. Gibson***
13:40 – 1340. Surprising role of uranyl peroxide in yellowcake drum pressurization. **P.C. Burns**
14:10 – 1341. Uranyl(V) cation-cation compounds with new topologies and single molecule magnet behaviour. **M. Mazzanti***
14:40 – 1342. Theoretical studies on coordination structures and electronic spectra of actinyl complexes. **J. Su***, J. Li*
15:10 Break
15:25 – 1343. Chemical predictive modeling in actinide chemistry. **P. YANG**
15:45 – 1344. Linking atomic structures of metal-ion complexes with their thermodynamic stability constants. **L. Soderholm***
16:15 – 1345. Water adsorption on AnO₂ (An = U, Pu) surfaces. J. Wellington, A. Kerridge, N. Kaltsoyannis*

16:45 – 1346. Basic studies on properties of uranyl(VI) species in ionic liquids as reaction media in nuclear fuel cycle. **Y. Ikeda***

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62)

Organized by: H. Kageyama, B. Kennedy, J. Wiley
Presiding: C. Brown, L. Chen, H. Kageyama, H. Karunadasa

13:00 Opening remarks
13:05 – 1347. Various structural polytypes and thermoelectric properties of layered tellurides Mo_{1-x}Nb_xTe₂. K. Ikeura, M. Bahramy, H. Sakai, **S. Ishiwata***
13:25 – 1348. Materials design using PTFE as an active deintercalation reagent. **T.C. Ozawa***, T. Sasaki
13:45 – 1349. Driving solid state reactions by controlling local environments. **M. Bieringer***
14:20 – 1350. Low-temperature synthesis of corundum-like Ti₂O₃ nanoparticles showing the insulator-metal transition. **Y. Tsujimoto***
14:40 – 1351. Deep ultraviolet NLO materials: Synthesis, structure, and characterization. **S. Halasayani**, T. Thanh, H. Yu, W. Zhang
15:00 Break
15:05 – 1352. Oxide-ion conduction in brownmillerite and perovskite Sr₂ScGaO₆. **N. Ichikawa***, S. Corallini, M. Ceretti, W. Paulus, Y. Shimakawa
15:25 – 1353. Impact of local structure on transparent conductors. **K.R. Poepelmeier***, K. Rickert
16:00 – 1354. Structural, electrical, and magnetic phase transitions in AX-type mixed valence cobalt oxynitrides epitaxial thin films. **Y. Hirose***, J. Takahashi, D. Oka, S. Nakao, C. Yang, T. Fukumura, T. Hasegawa
16:20 – 1355. Deposition of thermoelectric alkaline earth hexaboride thin films with MBE and CVD. **T. Tynell**, T. Aizawa, I. Ohkubo, T. Mori*

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Recent Discoveries in the Chemistry of Bismuth and Related Elements: the Green Alternative (#93)

Organized by: K. Whitmire, H. Sun, P. Andrews
Presiding: H. Sun

13:00 – 1356. Exploration of the coordination chemistry of bismuth carboxylates. **K. Whitmire***, I. Kumar, T. Boyd, E. Wagner
13:30 – 1357. One pot synthesis of triphenylbismuth(V) carboxylates. **I. Kumar***, K. Whitmire
13:55 – 1358. Pentavalent organobismuth compounds: Synthesis, structures, and applications to organic synthesis. **Y. Matano***

14:25 – 1359. Electrophilic antimony(V) derivatives. **F.P. Gabai**
14:55 Break

15:10 – 1360. Synthesis of highly functionalized triarylbismuthanes by functional group manipulation and use in C-, N-, and O-arylation reactions. **A. Gagnon**
15:35 – 1361. Modern twist to a classic synthetic route: Ph₃Bi-based redox transmetalation protolysis (RTP) for the preparation of alkaline earth metalorganic species. **K. Ruhiandt-Senge**, Y. Takahashi, A.g. Torvisco, A.Y. O'Brien, M.M. Gillett-Kunnath, G. Deacon, P. Andrews

16:00 – 1362. Dibismuthine reagents for efficient one-pot cross-coupling reactions. **S. Shimada***, X. Wang

16:30 – 1363. Chromium carbonyl complexes with tetrahedral and trigonal-planar coordinated bismuth. **M. Sheh***, K. Hsing, C. Yu

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Coordination and Supramolecular Chemistry for Aqueous Metal Ion Separations (#97)

Organized by: R. Ellis, D. Robinson, R. Motokawa

13:00 – 1364. Green chemistry principles applied to selective metal separations in metal processing and recovery using molecular recognition technology. **R.M. Izatt***

13:25 – 1365. Using the inner and outer coordination sphere to tune the strength of phenolic pyrazole extractants. **J.W. Roeckebuck, M.R. Healy, E. Doidge, V. Cocalia, A. Fischmann, J. Love, C.A. Morrison, T. Sassi, P. Tasker***

13:50 – 1366. Utility of short peptides in the separation of trivalent actinides from trivalent lanthanides. **T.S. Grimes***, P.R. Zalupska

14:15 – 1367. Extraction and structural properties of rhodium chloride complexes with amide-containing tertiary amine compounds. **H. Narita***, K. Morisaku, M. Tanaka, R. Motokawa, H. Shiwaku, T. Yaita

14:40 – 1368. Design of well-defined ligands for selective extraction of gold from low-grade gold ore using a simultaneous leaching and solvent extraction system: A viable alternative to the cyanide process. **S.R. Foley***

15:05 Break

15:20 – 1369. New opportunities for ion exchangers in hydrometallurgy. **J. Vaughan***

15:45 – 1370. Recent advances in palladium recovery: Application of coordination chemistry on an industrial scale. **R.J. Gordon***, R.A. Grant

16:10 – 1371. Investigating the interactions influencing chloroplatinate extraction by amidoether and amidamine reagents. **J. Love***, P. Tasker, C.A. Morrison, R.J. Gordon, R. Grant, E. Doidge, K. MacRuary, I. Carson, m. Wilson

16:35 – 1372. Development of new amides for lanthanide extraction and separation. **M. Tyumentsev**, M. Gergoric, M. Foreman, T. Retegan, B. Steenari, C. Ekberg

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

Frontiers of Molecular Magnetism (#109)

Organized by: H. Oshio, J. Miller, R. Oakley, S. Brooker, S. Gao, M. Ohba
Presiding: S. Brooker, E. Coronado

13:00 – 1373. Spin-crossover framework materials. **C. Kepert***

13:30 – 1374. Hofmann-like spin crossover coordination polymer compounds with 4-Xpyridine ligands. **T. Kitazawa***

13:50 – 1375. Spin crossover phenomena in polyanionic molecular Fe(II) complexes with polysulfonated-1,2,4-triazole. **J. Galan-Mascaros***, C. Saenz de Pipaon, P. Maldonado-Illescas, V. Gomez

14:10 – 1376. Creating a novel four-coordinated metal complex having spin cross-over phenomenon by means of distortion of molecule. **T. Ishii***, M. Nakano, M. Iwakura, K. Ogasawara, G. Sakane, M. Yamashita
14:30 – 1377. From octahedral to trigonal prismatic: New geometry and new magnetism for manganese(III). **G.G. Morgan***
14:50 Break

15:05 – 1378. Structure-property studies in photoresponsive cyanometalates. **S.M. Holmes**

15:25 – 1379. Hetero-spin chain exhibiting synergy between spin-crossover and magnetic coupling tuned by light, pressure, and hydration. **T. Liu**

15:45 – 1380. Rational design of photomagnetic chains with spin crossover complexes. **C. Mathoniere***, R. Ababel, A. David, R. Clerac, C. Pichon

16:05 – 1381. Novel optical functionalities in cyano-bridged metal assemblies. **S. Ohkoshi***

16:25 – 1382. Optical and magnetic molecular switches from solid state to solutions. **E. Koumousi, I. Jeon, D. Mitcov, D. Siretanu, P. Dechambenoit, C. Mathoniere, R. Clerac***

16:55 Closing Remarks

Hilton Hawaiian Village
Rainbow Tower, Rainbow 1

Electron Transfer and Electrochemistry of Inorganic and Organometallic Materials (#126)

Organized by: H. Nishihara, P. Harvey, W. Wong
Presiding: A.S. Abd El-Aziz, P.D. Harvey

13:00 – 1383. Ultrafast electron transfers (fs) within host-guest assemblies of mono-, Di-, and tetracarboxylate(meso-tetraphenylzinc(II)porphyrin and Pd³⁺(dpmp)₃CO)²⁺ as a model for TiO₂ in DSSC's. **P.D. Harvey***

13:30 – 1384. Insight into molecular electronics: Marcus theory to explain the diode properties in dye-sensitized solar cell. **N. Satoh***

* Principle Author

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13:50 – 1385. Construction of photo-responsive devices via the molecular conjugation at a surface. **K. Kanazuka***

14:20 – 1386. Zinc dipyrromes: Symmetry-breaking charge transfer and application to organic photovoltaics. **P.I. Djurovich***, S.E. Bradford, M. Thompson

14:40 – 1387. Charge transfer between colloidal amorphous TiO₂ nanoparticles and ZnO nanocrystals. **R. MITSUHASHI***, J. Lora, J. Mayer

15:20 – 1388. Transition metal aqueous solutions and aggregation complex formation: A photoelectron study. **R. Seidel***, M. Pohl, I. Unger, R. Golnak, K. Atak, K. Schulz, R. Kraehnert, A. Kabelitz, F. Emmerling, S. Thürmer, E. Aziz, B. Winter

15:20 – 1389. Design and electrochemical behaviour of cationic organolion dendrimers. **A.S. Abd-El-Aziz***, C. Agatemor, A.A. Abdelghani, B. Thabet, N. Etkin, R. Bisessur

15:50 – 1390. Redox bistability of a porphyrin in a supramolecular assembly of a porphyrin and a phthalocyanine joined with fourfold rotaxane. **Y. Yamada**, Y. Ishikura, K. Tanaka*

16:10 – 1391. Cyclometalated Ni(II) complexes [(Phbpy)NiX] (Phbpy' = 6-[(Phenyl-2-ide)-2',2'-bipyridine; X = various ligands). **A. Klein**

16:30 – 1392. Functionalized Ag₂S molecular architectures: Facile assembly of atomically precise, ferrocene-decorated nanoclusters. **J.F. Corrigan***, Y. Liu, B. Khalili Najafabadi, M. Azizpoor Fard

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Current Trends and Interconnectivities Among Fundamental and Applied Inorganic Fluorine Chemistry (#156)

Organized by: K. Matsumoto, R. Hagiwara, G. Schrobilgen, H. Mercier, R. Syvert
Presiding: G.J. Schrobilgen

13:00 Opening Remarks

13:05 – 1393. Computational studies of main group and metal fluorides: What can fluoride affinities tell us? **D.A. Dixon***, K.O. Christe

13:35 – 1394. Mixed noble-gas compounds: coordination of KrF₂ to Xe(VI) centers. **M. Lozinsek**, H.P. Mercier, G.J. Schrobilgen*

14:05 – 1395. Reactivity of selected pnictogen trifluorides. **G. Tavcar***, B. Alic, E. Goreshnik

14:35 – 1396. Surprises in the search for copper(I) fluoride. **F. Kraus***, A.J. Karttunen, P. Woidy

14:55 Break

15:10 – 1397. Synthesis and characterization of organylimidotungsten(VI) fluorides. **M. Gerken***, D. Turnbull

15:40 – 1398. Synthesis of fluoroalkylamines and -ammonium salts by HF addition across C'N bonds. R. Haiges, A. Baxter, K.O. Christe*

16:10 – 1399. Combustion properties of 2,3,3,3-tetrafluoropropene (HFO-1234yf). **A.J. Kornath**, C. Hohenstein, M. Feller, F. Zischka

16:30 – 1400. Structure and properties of carbonyl fluoride. **M. Feller***, A.J. Kornath

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170)

Organized by: K. Theopold, K. Mashima, Z. Xie
Presiding: M. Tamm

13:00 – 1401. Dittanoxycarbene: Coordination and reactivity of the carbon dioxide dianion. **J. Okuda***

13:30 – 1402. Syntheses, characterization, and reactivity of vanadium(V) complexes with a bis(hydroxyethyl)pyridine backbone. **Y. Kajita***, D. Arakawa, H. Masuda

13:50 – 1403. Activation of O₂ for one- and two-electron reactivity using tantalum(V) complexes. **A. Heyduk***, A. Hollas

14:20 – 1404. Cationic alkylhafnium complexes supported by nitrogen-based multidentate ligands as catalysts for hydroalkylation of internal alkynes via C(sp³)-H activation of 2-methylpyridines.

M.J. Lopez, A. Kondo, K. Yamamoto, H. Tsurugi*, K. Mashima*

14:40 – 1405. Isoselective polymerization of propylene by group 4 complexes of sequential tetradentate ligands. **M. Kol***, K. Press, V. Venditto, I. Goldberg

15:10 – 1406. C-H activation processes involving s-alkyl titanocene complexes.

M.C. Baird, A. Dunlop-Brière, P.H. Budzelaar

15:30 – 1407. Unexpected stability of di-nuclear alkyl hydrides of chromium.

Y. Hung, L. Wang, G.P. Yap,
K.H. Theopold*

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

Photofunctional Chemistry Based on Metal Complexes and/or Supramolecules (#239)

Organized by: K. Ishii, Z. Chen, P. Ford, G. Hanan

13:00 – 1408. Photofunctional approach to artificial photosynthesis. **s. campagna**, F. Puntoriero, F. Nastasi, G. La Gangà, S. Serroni, M. Galletta

13:25 – 1409. Unique photo-functions of Rub(ppy)₃²⁺ on clay surface. **T. Yui**

13:40 – 1410. Self-assembly of coordination polymers based on POMs: Design, synthesis, and photocatalytic property.

H. Zhang
13:55 – 1411. Supramolecular ruthenium complexes bridged with peptides for photochemical CO₂ reduction catalysts.

H. Ishida*
14:20 – 1412. Light-harvesting host: Photoisomerization of anthracene derivatives in the cavity of Ru square by visible light irradiation. **M. Yamaguchi***, R. Moriyama, A. Hirayama, M. Obara, K. Sato

14:35 – 1413. Enhancement of polymer bulk heterojunction solar cells using triplet-singlet energy transfer. **T. Kwon***

14:50 Coffee Break

15:00 – 1414. Homogenous approaches to solar hydrogen photocatalysis.

F.N. Castellano*

15:25 – 1415. Chemical and electrochemical control of emission colour in electrochemiluminescent systems. **C.F. Hogan***, P. Francis

15:40 – 1416. Dynamics of nuclearity conversion reactions of photo-emissive multinuclear pyridinethiolato Cu(I) complexes in solution. **Y. Ozawa***, M. Kubo, A. Nagasaki*, K. Toriumi

15:55 – 1417. Controlling photophysical properties of π -conjugated oligomers with metal complex and Lewis-pair interactions.

M.O. Wolf, Y. Cao
16:10 – 1418. Phosphorescent d⁸-d¹⁰/d¹⁰-d¹⁰ heterometallic alkynyl complexes for Organic Light-Emitting Diodes. **F. Dai***, L. Zhang, L. Xu, Z. Chen*

16:25 – 1419. ESIPT-based photoluminescent coordination complexes: Potentials in chemical sensing and electroluminescent devices.

M. Pan
16:40 – 1420. Synthesis of a luminescent, redox active, mixed metal Os₄Cd₄ coordination cage.

A. Wragg*, M. Ward
16:55 Concluding remarks

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2

Inorganic Complexes for Solar Energy Harvesting (#256)

Organized by: M. Wolf, K. Sakai, F. MacDonnell
Presiding: K. Sakai

13:00 – 1401. Dittanoxycarbene: Coordination and reactivity of the carbon dioxide dianion. **J. Okuda***

13:30 – 1402. Syntheses, characterization,

and reactivity of vanadium(V) complexes with a bis(hydroxyethyl)pyridine back-

bone.

Y. Kajita*, D. Arakawa, H. Masuda

13:00 – 1421. Electrochemical reduction of CO₂: Hydricities and reduction potentials control switching between CO₂ reduction to formate, CO₂ reduction to CO, and formate oxidation.

C. Machan, A. Lilio, M. Reineke, **C.P. Kubik***

13:35 – 1422. Quantitative measurements of hydride donor ability and application towards new electrocatalysts for reduction reactions.

J.Y. Yang*

14:10 – 1423. Deep photoreduction of carbon dioxide and formate to methanol by ruthenium poly(pyridyl) chromophores with pendant pyridyl reduction sites.

F.M. MacDonnell, M.J. West, N.S. de Tacconi

14:30 – 1424. Some excited-state properties that relate to the design of efficient transition metal solar photosensitizers.

R.A. Thomas, C. Tsai, S. Mazumder, Y. Chen, H.B. Schlegel, **J.F. Endicott***

14:50 Break

15:05 – 1425. Photochemical and electrochemical reduction of a low concentration of CO₂.

O. Ishitani

15:40 – 1426. Working the other way around: Photocatalytic water oxidation triggered by reductive quenching of the photosensitizer.

s. campagna*, F. Puntoriero, F. Nastasi

16:15 – 1427. Mechanisms of molecular solar fuels catalysts.

L. Hammarström*

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

Metal Mediated Polymerization (#292)

Organized by: P. Hayes, R. Waterman, T. Mizuta, Y. Tang, P. Sanghirutnugul
Presiding: L.L. Schafer, R. Waterman

13:00 – 1428. Importance of being (diastereomerically) earnest - mechanistic insight into ring-opening polymerization catalysts.

M. Kol*, K. Press, V. Venditto, M. Lamberti, I. Goldberg

13:30 – 1429. Amino-phenoletol complexes of earth abundant metals in polymerization catalysis.

F. Kerton, D. Alhashmialameer, H. Plommer, A. Elkurtehi, S. Chowdhury, K. Hattenauer

14:00 – 1430. Versatile iron-based catalysts for the control of tacticity, architecture, and composition in biodegradable polymers.

J.A. Byers*, A.B. Biernesser, C.M. Manha, K. Delle Chiaie, A. Kaur, J. Kehl, H. Borland, J. Curley

14:20 – 1431. Cationic zinc lactide polymerization catalysts supported by extremely sterically demanding NON pincer ligands.

P.G. Hayes*

14:50 Intermission

15:00 – 1432. Synthesis of cyclic polyesters:

The catalyst design.

P. Wongmahasirikun, P. Prom-on,

K. Phomphrai*

15:30 – 1433. Coupling and copolymerization of epoxides and CO₂ using transition metal catalysts.

C.M. Kozak*,

K. Pressing-Devaire, H. Chen, K. Ni,

K. Ambrose

16:00 – 1434. Catalysis of cyclic ester polymerization using manganese, iron or copper complexes.

F. Schaper,

P. Daneshmand Kashani, T. Whitehorne,

A. Keuchguerian

16:30 – 1435. Unorthodox main group precatalysts for ring-opening polymerizations: Design and mechanisms.

Y. Sarazin*,

J. Carpenter, M. Bochmann

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Metal Coordination Sphere Design for Challenging Bond Transformations (#318)

Organized by: K. Caulton, A. Hill, S. Johnson, M. Yamashita
Presiding: L.L. Schafer, M. Yamashita

13:00 – 1436. Non-innocent PNP-pincer

type phosphalkene ligands: A powerful

tool for metal-ligand cooperative activation of inert molecules.

F. Ozawa

13:20 – 1437. Low-valent low-coordinate iron and cobalt complexes with NHC ligation: Synthesis, structure, and reactivity.

L. Deng*

13:40 – 1438. CH activation and aerobic functionalization at the same metal center and in the same system.

A. Vedernikov*

13:55 – 1439. Molybdenum-atalyzed reduction of molecular dinitrogen into ammonia under ambient conditions.

Y. Nishibayashi*

14:15 – 1440. Density functional study of rhodium(I) o-complexes in the solid-state.

T. Kraemer, M. Chadwick, S. Pike, A.S. Weller*, S.A. Macgregor*

14:30 – 1441. Non-innocent ligand complexes support water as an oxidant for alcohols: Computational studies of the catalytic mechanisms.

M. Hall, H. Li

14:45 – 1442. Cooperative catalysis using homobimetallic and heterobimetallic complexes.

B.A. Messerle*, M. Gatus, S. Choy, M.B. Peterson, A.G. Nair, D.B. Walker

15:05 – 1443. Selective dehydrogenative coupling of alcohols and hydrogenation of esters.

D.G. Gusev*

15:25 – 1444. Harnessing metal-metal bonds for cleaving small molecules.

C. Lu

15:45 – 1445. Transition metal coordination to acyclic conjugated tri-pi hydrocarbons: edienynes, dienyne, and trienes.

J.M. O'Connor*, S.K. Cope, D.M. Hitt, K.K. Baldridge, S.J. Fries, A.L. Rheingold, C. Moore

16:00 – 1446. Tantalum phosphinidene complexes: Synthesis and reactivity.

E. Hey-Hawkins*, A. Grundmann, P. Lönnecke

16:15 – 1447. Optically active inorganophosphorus chelates for asymmetric catalysis.

K.F. Smith*, D. Norman, C.L. McMullin, P.G. Pringle

16:30 Flash 4

Friday Evening

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson, G. Schreckenbach, T. Yaita, J. Li, P. Yang
Presiding: J. Li

19:00 – 1448. Studying some of the unusual oxygen behavior in the fluorite based metal oxides — mechanisms and kinetics of the oxygen exchange reaction on $^{238}\text{PuO}_2$, $^{241}\text{AmO}_2$, and CeO_2 .

C.E. Whiting*, M. Du, L.K. Felker, R.M. Wham, C.D. Barklay, D.P. Kramer

19:20 – 1449. Ionothermal synthesis of UO_2^{2+} and NpO_2^{2+} coordination compounds using task-specific ionic liquids.

P.A. Smith*, P.C. Burns

19:40 – 1450. Hydrolysis and condensation process of tetravalent uranium in aqueous solution.

C. Falaise, M. Nyman

20:00 – 1451. Theoretical investigation of λ -type pre-melting transition in thorium.

B. Szpunar*, J. Szpunar

* Principle Author

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102-TECH

- 20:20 – 1452.** Phenanthrolineamide functionalized mesoporous KIT-6 for selective U(VI) uptake: An experimental and theoretical investigation. L. Zhu, C. Xiao, L. Yuan, W. Shi*, Z. Chai
20:40 – 1453. Computational study on the chemical separation of Am(III) from Eu(III) by means of scalar relativistic density functional theory. M. Kaneko*, S. Miyashita, S. Nakashima

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

Metal-Organic Frameworks: Synthesis, Properties and Applications (#50)

Organized by: G. Shimizu, J. Long, M. Suh, Q. Xu, X. Chen

- 19:00 – 1454.** Porous stable metal organic frameworks for applications in energy and environment. c. SERRE*, G. Maurin, M. Daturi

- 19:30 – 1455.** Developing solid-state reactivity for the discovery and clean, high-yielding synthesis of metal-organic frameworks. T. Frisch*

- 19:50 – 1456.** Coordination assembly of porous solid materials incorporating functional sites or groups. C. Su

- 20:10 – 1457.** Microporous metal-organic frameworks for separation of C2H2/C2H4. B. Chen*

- 20:30 – 1458.** Cationic metal-organic frameworks for reversible anion trapping. S. Oliver*

- 20:45 – 1459.** Encapsulation of red sulfur chromophores in zeolitic imidazolate framework (ZIF-8) by SALE. K. Balkus*, S. Basnayake, K. Tan, Y. Chabal

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62)

Organized by: H. Kageyama, B. Kennedy, J. Wiley
Presiding: M. Azuma, R. Seshadri

- 19:00 – 1460.** Exploration of novel chalcogenides and their nonlinear optical properties. L. Chen

- 19:35 – 1461.** Prospectives for enhancing thermoelectric materials by utilizing principles based on structural features in borides. T. Mori

- 20:10 – 1462.** Magnetic and thermoelectric properties new antimonide with CaAl₂Si₂-type structure. T. Murakami, T. Yamamoto, H. Kageyama

- 20:25 – 1463.** Structural chemistry and physical properties of fluorine-substituted perovskite nickelate NdNiO_{3-x}F_x thin films. T. Onozuka, A. Chikamatsu, T. Katayama, T. Fukumura, T. Hasegawa*

Hawaii Convention Center
Halls I, II, III

Chemistry and Application of Boron Clusters (#152)

Organized by: S. Kang, N. Hosmane, D. Schubert, H. Nakamura, Z. Xie
Presiding: S. Kang

Poster Session
19:00 – 21:00

- 1464.** Introduction of aromatic rings into C1-carborane anion and their properties. M. Otsuka, J. Kanazawa, R. Takita, M. Uchiyama

- 1465.** o-Carborane dyads for low-energy photosensitization. Y. Cho, S. Kim, A. Lee, H. Son*, W. Han, S. Kang

- 1466.** Synthesis and photophysical properties of iridium(III) cyclometalates with restricted rotation of o-carborane. Y. Lee*, J. Park, H. Lee, M. Lee

- 1467.** Design and synthesis of new boron carriers based on pepducin chemistry and evaluation of their subcellular distribution. A. Isono, H. Terashima, S. Masunaga, T. Hirayama, K. Okuda, H.K. Nagasawa

- 1468.** Photochemistry of hybrid organic-inorganic triarylborane-o-carboranes. S. Kim, J. Lee, H. Son, W. Han*, S. Kang

- 1469.** Use of serum albumin as an efficient boron delivery carrier for neutron capture therapy. S. Kikuchi, D. Kanoh, S. Sato, H. Nakamura*

- 1470.** Electronic alteration on oligothiophenes by o-carborane. S. Kim, Y. Cho, J. Lee, H. Son, W. Han, S. Kang*

Hawaii Convention Center
Halls I, II, III

Current Trends and Interconnectivities Among Fundamental and Applied Inorganic Fluorine Chemistry (#156)

Organized by: K. Matsumoto, R. Hagiwara, G. Schrobilgen, H. Mercier, R. Syvert
Presiding: H.P. Mercier

Poster Session

19:00 – 21:00

- 1471.** [XeF₅]⁺ and [Xe₂F₁₁]⁺ salts of the [Cr^VF₅]²⁻, [Cr^VOF₅]²⁻, [Cr₂V₂O₂F₅]²⁻, [Mo^{VI}OF₅]⁻, and [Mo₂V₂O₅]⁻ anions. J.T. Goettel, D.G. Stuart, H.P. Mercier, G.J. Schrobilgen*

- 1472.** Squamic acid in super acids. M.T. Schickinger*, A.J. Kornath

- 1473.** Synthesis and reactivity of metal fluorocarbene complexes. G.M. Lee*, R. Baker*

- 1474.** Protonation of malononitrile. Y. Morgenstern*, M.T. Schickinger, A.J. Kornath

- 1475.** Protonation of methylphosphonic acid. E.E. Erhardt*, Y. Morgenstern, A.J. Kornath

- 1476.** Crystal structures of chloroufonamide and its protonated species as hexafluoridorgermanate salt. D. Leitz, Y. Morgenstern, A.J. Kornath

- 1477.** Effects of the surface fluorination on the electrochemical properties and thermal stability of LiFePO₄ cathode material. K. Degura*, J. Kim, S. Yonezawa, M. Takashima

- 1478.** Surface fluorination and cobalt coating of Li_{0.5}Mn_{1.5}O₄ spinel cathode for Li-ion battery. K. Ura

- 1479.** Preparation and electrochemical characterization of Li₄Ti₅O₁₂ using surface-fluorinated TiO₂. M. Kohno*, J. Kim, S. Yonezawa, M. Takashima

- 1480.** Effects of surface fluorination on the synthesis process of LiNiO₂ as a cathode active material for lithium ion batteries. S. Yamada*, J. Kim, S. Yonezawa, M. Takashima

- 1481.** Chemical state analysis of various fluorides by using AES. F. Nishimura, J. Kim, S. Yonezawa, M. Takashima

- 1482.** Preparation and characterization of CaSiO₃ particles with fluorinated SiO₂. K. Maekawa*, J. Kim, S. Yonezawa, M. Takashima

Hawaii Convention Center
Halls I, II, III

Activation and Transformation of Small Molecules Mediated by Early Transition Metal Complexes (#170)

Organized by: K. Theopold, K. Mashima, Z. Xie

Poster Session

19:00 – 21:00

- 1483.** Construction of spiro skeleton with titanocene complex. M. Bando, Y. Mizukami, Z. SONG, K. Nakajima, T. Takahashi*

- 1484.** Synthesis and catalytic activity of dimolybdenum-dinitron complex bearing PCP-type pincer ligands. A. Eizawa, K. Arashiba, S. Kuriyama, K. Nakajima, Y. Nishibayashi*

- 1485.** Synthesis and reactivity of zirconocene complexes with bidentate phosphine ligands. M. Hosoya, Y. Ariga, Y. Masuyama, N. Suzuki*

- 1486.** Salt-free reduction of niobium imido complex by organosilicon reductants and their reactivity toward N=N bond. K. Kawakita, T. Saito, H. Nishiyama, M. Nechayev, B.M. Kriegel, H. Tsurugi, J. Arnold, K. Mashima*

- 1487.** Synthesis of stable five-membered cycloallole complexes that contain a sulfur atom and Group 4 metal. A. Kawamura, T. Asada, Y. Masuyama, N. Suzuki*

- 1488.** Synthesis five-membered zirconacycloalleenes and their reactions to form allenyl alcohols. R. Kurita, M. Hosoya, Y. Masuyama, N. Suzuki

- 1489.** Synthesis of substituted metallocene complexes. H. Nakata, Z. SONG, K. Nakajima, T. Takahashi*

- 1490.** Titanium Lewis acid mediated asymmetric synthesis of hydroxylamines via alkylation of O-diphenylphosphoryl oxime substrates. J.M. Tanski*, S.H. Majer, B. Zhang

- 1491.** Imidophosphorane group VI complexes containing metal-element multiple bonds. C. Varjas, R.K. Thomson*

Hawaii Convention Center
Halls I, II, III

The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NO_x Generation, Signaling and Reduction in Biological Systems (#371)

Organized by: N. Lehner, G. Richter-Addo, F. Doctorovich, K. Fujisawa

Poster Session

19:00 – 21:00

- 1492.** Four-coordinate nickel nitrosyl complexes supported by a PEP ligand: Tetrahedral vs. square planar geometry. J. Gwak, Y. Kim, Y. Lee*

- 1493.** Modeling the key intermediate in cytochrome P450 nitric oxide reductase: Electronic structure and reactivity. A. McQuarters*, N. Lehner

- 1494.** First structurally determined (FeNO)⁸ porphyrin complex. J. Li*

- 1495.** Nitric oxide production by *Trichomonas vaginalis*. K.D. Jordan, N. Yarlett, R.K. Upmacis*

- 1496.** Characterization of a high-spin non-heme [FeH(HO)]³⁻: Implications for the reactivity of iron nitroxyl species in biology. A.L. Speelman, N. Lehner

- 1497.** Spectroscopic characterization of iron-nitroxyl intermediates in heme-non-heme diiron center of engineered denitrifying nitric oxide reductase mode.

- 1498.** H. Matsumura, S. Chakraborty, Y. Lu, P. Moënne-Loccoz

- 1499.** Reactivity study of a five-coordinate cobalt complex with nitric oxide. C. Wang, W. Lee*, W. Liaw*

- 1500.** Syntheses, structures, and electrochemical studies of bioinspired iron nitroxyl complexes. L. Li*

- 1501.** Synthesis and spectroscopic characterization of ferric heme-thiolate complexes as models for cytochrome P450 nitric oxide reductase. A.P. Hunt*, N. Lehner

Saturday Morning

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson, G. Schreckenbach, T. Yaita, J. Li, P. Yang

Presiding: M.A. Denecke, S. Tsuchima

- 8:00 – 1501.** Behavior of AmVI in nitric acid solution: Preparation, complexation, and autoxidation. B.J. Mincher*, T.S. Grimes, C.C. Dares, N.C. Schmitt

- 8:20 – 1502.** From hydrogen to neptunium: Uranyl oxo-functionalisation by as much of the periodic table as possible. P.L. Arnold*, M. Zegke, G. Jones, A. Pechmann, R. Lord, E. Hollis, M. Dutkiewicz, J. Love, R. Caciuffo, N. Magnani, C. Apostolidis, O. Walter, X. Zhang, G. Schreckenbach, I. Pidchenko, T. Vito

- 8:50 – 1503.** Californium: The second tipping point in the actinide series. T.E. Albrecht-Schmitt*

- 9:20 – 1504.** Modulation of interfacial properties in liquid/liquid solvent extraction via solution phase conditions: The role of organic diluent, ionic strength, and amphoteric solutes. A.E. Clark

9:50 Break

- 10:05 – 1505.** Probing the electronic structure and chemical bonding in mononuclear uranium oxides (UO_x⁻, x = 1–5) using photoelectron spectroscopy. L. Wang*

- 10:35 – 1506.** Biomimetic ligand platforms for specific recognition and enhanced luminescence sensitization of actinides.

- R.J. Abergel*, M. Sturzbecher-Hoehne, B. Allred, P. Rupert, P. YANG, A. D'Aléo, R. Strong

- 11:05 – 1507.** Ab initio thermochemistry and spectroscopy for molecules containing f-block elements. K.A. Peterson*

- 11:35 – 1508.** Actinide ion recognition mechanism by organic ligands. T. Yaita*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

Metal-Organic Frameworks: Synthesis, Properties and Applications (#50)

Organized by: G. Shimizu, J. Long, M. Suh, Q. Xu, X. Chen

8:00 Opening remarks

- 8:05 – 1509.** New opportunities in the field of metal-organic frameworks. O.M. Yaghi

- 8:35 – 1510.** Combined experimental, theoretical, and computational approach to redox-active metal-organic frameworks. D.M. D'Alessandro*, C.F. Leong, P.M. Usov, B. Chan

- 8:55 – 1511.** Applications of functional metal-organic frameworks. Q. Xu

- 9:15 – 1512.** Tetravalent MOFs as catalysts for oxidation and esterification reactions. D. De Vos*

- 9:35 – 1513.** Biomimetic mineralization of metal-organic frameworks and its potential in biotechnology. K. Liang*, P. Falcaro

- 9:50 – 1514.** Luminescent metal-organic frameworks and related applications. J. Li*

- 10:10 – 1515.** Porous metal-organic materials for gas storage and selectivity. S. Yang*

- 10:30 – 1516.** Flexibility and functionality in metal-organic frameworks. S. Kaskel

- 10:50 – 1517.** Crystal engineering of hybrid ultramicroporous materials. M. Zawortko*

- 11:10 – 1518.** Highly porous medical metal-organic framework constructed from bioactive curcumin. G. Zhu

- 11:30 – 1519.** Lanthanide-organic frameworks for optical sensing and nanothermometry. J. Rocha*

*** Principle Author**

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TECHNICAL PROGRAM

Hilton Hawaiian Village

Mid-Pacific Center, South Pacific Ballrm 2

From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62)

Organized by: H. Kageyama,
B. Kennedy, J. Wiley
Presiding: Z. Hiroi, C.D. Ling, Y. Liu,
K. Ok

8:00 – 1520. Understanding and prediction of multiferroics. **H. Xiang**

8:35 – 1521. A-site magnetism in the Mn-spin sublattice of A-site ordered perovskites $AMn_3Ba_2O_{12}$. **T. Saito***,
S. Zhang, M. Toyoda, T. Oguchi,
C. Ritter, J.P. Atfield, Y. Shimakawa

8:55 – 1522. Itinerant (3d) ferromagnetism in ACo_2As_2 ($A = Eu, Ca$) induced by localized (4f) valence fluctuations. X. Tan,
G. Fabbri, D. Haskel, A. Yaroslavtsev,
M. Shatruk

9:15 – 1523. Enhancement of superconductivity by La and Sb double doping of 112-type iron pnictide $CaFeAs_2$. **M. Nohara***,
Y. Kitahama, K. Fujimura, T. Mizukami,
K. Kudo

9:35 – 1524. Superconductivity and magnetism in solution-produced FeSe-based material. **K. Kovnir**

9:55 Break

10:05 – 1525. Superconductivity in titanium pnictide oxides. **T. Yajima***, K. Nakano,
F. Takeiri, Y. Nozaki, W. Ishii, Z. Hiroi,
T. Ono, Y. Hosokoshi, Y. Matsushita,
J. Hester, T. Yamamoto, N. Tsuji, J. Kim,
A. Fujiwara, Y. Kobayashi, H. Kageyama

10:25 – 1526. Collapse transition in early transition metal pnictide. **T. Yamamoto***,
T. Kawakami, T. Yajima, T. Okada,
H. Kageyama

10:45 – 1527. Local structure effects in functional materials. Examples of lighting phosphors, magnetic, and thermoelectric materials. **R. Seshadri**

11:20 – 1528. Structure of BiS_2 Layer in $Bi_4O_4S_3$. **A. Miura***, Y. Mizuguchi,
T. Sugawara, T. Takei, N. Kumada,
E. Magome, C. Moriyoshi, Y. Kuroiwa,
K. Tadanaga

11:40 – 1529. Effect of oxygen content in iron-pnictide superconductors with thick blocking layers. **H. Ogino***,
J. Shimoyama, K. Kishio

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2**Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications (#87)**

Organized by: T. Storr, C. Grapperhaus,
H. Fujii
Presiding: H. Fujii, T. Storr

8:00 – 1530. Radical-type catalytic reactions involving substrate radicals. **B. de Bruin***

8:30 – 1531. Highly-tunable donor-acceptor LL'CT complexes of the 3d metals.
A. Heyduk*, L. Cameron, E. Seraya

9:00 – 1532. Metal complexes of redox-active ligands for bond-activation reactions and catalysis. **B. Sarkar***

9:30 – 1533. Electronic structure and imidyl radical reactivity in chromium phenylene-diamido complexes. A. Mottier, W. Zhou,
G. Dilabio*, **K.M. Smith***

9:50 Break

10:00 – 1534. Redox switches for catalysis using ferrocene-based ligands.
P.L. Diaconescu

10:30 – 1535. C-H, C-C and C-N activation of redox-active pyridines in reduced iron complexes. R.A. Lewis, K.C. MacLeod,
B.Q. Mercado, **P.L. Holland**

11:00 – 1536. Oxidation chemistry of nickel(II)-di(phenolate) complexes.
Y. Shimazaki*

11:30 – 1537. Redox-active pincer ligands for Fe, Co and Ni catalyzed C-C cross coupling via C-O or C-H bond activation.
J.D. Soper*

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2**Recent Discoveries in the Chemistry of Bismuth and Related Elements: the Green Alternative (#93)**

Organized by: K. Whitmire, H. Sun,
P. Andrews
Presiding: K. Whitmire

8:00 – 1538. Bismuth chalcogenide chemistry from exploratory synthesis to compound prediction and a treasure trove of properties. **M.G. Kanatzidis***

8:30 – 1539. Magnetic properties of bismuth molecules and materials. S. Clarke,
S. Coste, **D.E. Freedman**

9:00 – 1540. Bismuth-rich materials: A perspective for electronics close to the atomic limit. **M. Ruck**

9:30 Break

9:45 – 1541. Solvent-free solid-state synthesis of bismuth salicylate complexes by accelerated aging and mechanochemistry. **D. Tan***, F. Qi, T. Frisic

10:15 – 1542. Mesmerizing chemistry of bismuth: Many happy returns. **E.V. Dikarev***

10:45 – 1543. New explorations into transition metal pnictide clusters.
D.E. Schipper, K. Whitmire

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4**Chemistry and Application of Boron Clusters (#152)**

Organized by: S. Kang, N. Hosmane,
D. Schubert, H. Nakamura, Z. Xie
Presiding: N.S. Hosmane

8:00 Introductory Remarks

8:00 – 1544. New carborane ligands and their σ - and π - metallococomplexes.
V.I. Bregadze*

8:30 – 1545. Synthesis and reactivity of novel carbonyne precursor 1-OTf-1,2- $C_2B_10H_{11}$. **Z. Qiu***

8:50 – 1546. Chemistry of carboranylaminides. N. Harmgarth, C.G. Hrib,
V. Lorenz, L. Hilpert, P. Dröse,
F. Edelmann

9:20 Break

9:30 – 1547. Coordination chemistry of carboranylaminide ligands. **G. Jin***

10:00 – 1548. Carborane based optoelectronically active materials. A. Lee, J. Lee,
J. Lee, **W. Han***

10:20 – 1549. Triple decker sandwich complexes incorporating six membered ring as middle deck. **S. Ghosh***

10:50 Break

11:00 – 1550. Intermolecular interactions involving boron hydrides clusters: Theory and experiment. **E. Shubina***

11:30 – 1551. Chemistry of bis(carboranes).
A.J. Welch

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2**Current Trends and Interconnectivities Among Fundamental and Applied Inorganic Fluorine Chemistry (#156)**

Organized by: K. Matsumoto,
R. Hagiwara, G. Schrobilgen, H. Mercier,
R. Syvert
Presiding: R. Hagiwara

8:00 – 1552. Recent attempts to improve the capabilities of commercial CFx to enhance the efficiency of Li/CFx batteries.
D.T. Meshri, E. Shembel , S.D. Meshri,
R.L. Adams , D. Pinnapareddy, V. Redko,
I. Maksyuta, A. Markevich , N. Mathur

8:30 – 1553. Improving life and safety of lithium ion batteries via fluorine based organic and inorganic coating of electrode materials. **K. Amine***

9:00 – 1554. Fluoride-phosphates of transition metals and Li/Na as perspective cathode materials for Li-ion batteries.

E. Antipov*, N. Khasanova, S. Fedotov,
O. Drozhzhin

9:30 – 1555. Surface fluorination of nickel containing cathode active materials for lithium ion battery. **S. Yonezawa**, J. Kim,
M. Takashima, J. Imaiizumi

9:50 – 1556. High substitution rate in TiO_2 anatase nanoparticles for high rate capability and modified lithium storage mechanism. **D. Dambourgen***, W. Li,
D. Corradini, M. Salanne, M. Body,
C. Legein, K. Chapman

10:10 Break

10:20 – 1557. Versatility of C-F bonding in fluorinated carbons. **M. Dubois***,

K. Guerin, Y. Ahmad, A. Hamwi, F. Masin,
A. Vinogradov

10:50 – 1558. Covalent attachment of perfluoroalkyl groups to layered materials.
Y. Matsuo*

11:20 – 1559. Effects of ion mixing on the structures and properties of ionic plastic crystals. **K. Matsumoto***, R. Nonaka,
R. Tanaka, R. Hagiwara

11:40 – 1560. Gradient surface modification of an electrode with fluoro-functionality by means of bipolar electrochemistry.
S. Inagi*, N. Shida, T. Fuchigami

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2**Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus, and Synthesis (#226)**

Organized by: R. Waterman, F. Ozawa,
D. Gates, P. Leung
Presiding: R.L. Webster

8:00 – 1561. Complexes with super-strained three-membered P-ligands: Synthesis and insights into substrate dependent reactivity. **R.K. Streubel***,
J. Villalba Franco

8:20 – 1562. Phosphino(boryl)carbenes and azavinylidenephosphoranes, two new type of push-pull carbenes.
A. Baceiredo*, E. MAERTEN, T. KATO

8:40 – 1563. Palladium-catalyzed hydrophosphorilation of alkynes: Scope, limitation, and mechanism. **L. Han***

9:00 – 1564. Inner- and outer-sphere roles of terminal ruthenium phosphido complexes in P-C bond formation. R.G. Belli,
S.A. Ruff, J. Yang, D. Pantazis,
R. McDonald, **L. Rosenberg***

9:20 – 1565. Organopalladium complex catalyzed asymmetric P-H addition reactions.
P. Leung*

9:40 – 1566. Activation of P_4 and preparation of novel types of phosphorus species.
G. Bertrand

10:00 – 1567. Reduction behavior of Fe(II) complexes bearing a PNP-pincer type phosphaalkene ligand. **Y. Nakajima**,
Y. Lin, N. Ichihara, F. Ozawa

10:20 – 1568. Transition-metal catalyzed reactions that form bonds to phosphorous.
R. Waterman

10:40 – 1569. Catalytic hydrosilylation of CO_2 using an iridium(I) complex bearing unsymmetrical PNP-pincer type phosphaalkene ligands. Y. Chang,
K. Takeuchi, F. Ozawa*

11:00 – 1570. Room temperature hydrophosphorilation using a simple iron salen pre-catalyst. K.J. Gallagher, C.A. Brown,
M.F. Mahon, **R.L. Webster***

11:20 – 1571. Catalytic asymmetric synthesis of phosphorus compounds. **W. Duan***

11:40 – 1572. Phosphine-participated C-H transformations. **S. Yang**

Hilton Hawaiian Village
Kalia Tower, Lehua Suite**The Expanding Periodic Table: New Discoveries and Chemistry of the Heaviest Elements (#234)**

Organized by: Y. Nagame, H. Nitsche,
Z. Qin, P. Schwerdtfeger, C. Duellmann,
A. Tueller
Presiding: C.E. Duellmann, Y. Nagame

8:00 – 1573. Search for new elements at TASCA at GSI. **K. Jadambaa***

8:30 – 1574. Synthesis of superheavy elements at RIKEN. **K. MORIMOTO**

9:00 – 1575. SHE factory: Current status.
G. Chubarion*

9:30 – 1576. Synthesis and nuclear structure studies of heavy elements with the Berkeley Gas-filled Separator. **K.E. Gregorich***

10:00 – 1577. Toward A and Z identification of superheavy elements. **J. Gates***

10:30 – 1578. Production and decay studies of ^{261}Pr , ^{265}Db , ^{265}Sg , and $^{266,267}Bh$ for superheavy element chemistry using GARIS at RIKEN. **H. Haber***

11:00 – 1579. Random probability analysis of recent $^{48}Ca + ^{238,240}Pu$ experiments for the production of flerovium.
M.A. Stoyer*, S. Strauss, Y. Oganessian,
F. Abdullin, R. Boll, N. Brewer,
S. Dmitriev, J. Ezold, L.K. Felker,
R. Grzywacz, J. Hamilton, R. Henderson,
M. Itkis, K. Miernik, A. Polyakov,
J. Roberto, K. Rykaczewski,
A. Sabelnikov, R. Sagaidak,
D. Shaughnessy, I. Shirokovsky,
M. Shumeyko, N. Stoyer, V. Subbotin,
A. Sukhov, Y. Tsyanov, V. Utyonkov,
A. Voinov, G. Vostokin

11:30 – 1580. Heavy element study using a new separator GARIS-II. **D. Kaji***,
K. MORIMOTO

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2**Advances in the Medicinal Applications of N-Heterocyclic Carbene Metal Complexes and Azolium Cations (#255)**

Organized by: W. Youngs, M. Baker,
C. Che, I. Lin, M. Panzner
Presiding: W. Youngs

8:00 Opening Remarks

8:10 – 1581. Development of novel silver-based antimicrobial formulations for the treatment of pulmonary infections.
P.N. Shah*, J.A. Smolen, J.A. Tagaev,
S. Zhang, F. Zhang, Y.H. Lim, G. Heo,
B. Wright, M.J. Panzner, W. Youngs,
K. Wooley, **C.L. Cannon**

8:45 – 1582. Assessment of the clearance and pharmacokinetics of silver antimicrobials using ^{113}Ag . T. Aweda, S. Zhang,
B. Wright, J. Burkemper, G. Heo,
N. Bandara, C.S. Cutler, C.L. Cannon,
W. Youngs, K. Wooley, **S.E. Lapi**

9:20 – 1583. Therapeutic polymer nanoparticle designed for treatment of pulmonary and urinary tract diseases.
K. Wooley

9:55 Break

10:10 – 1584. New routes to carbene-functionalized metal surfaces. **M.T. Zamora**,
C.A. Smith, M. Narouz, C. Crudden

10:45 – 1585. Beyond catalysis, the new horizon of the biomedical applications of the late-transition metal N-heterocyclic carbene complexes. **P. Ghosh***, D. Panda*

11:20 – 1586. Antimicrobial activity of silver N-heterocyclic carbene mediated self-assembling hydrogels based on the naturally occurring human peptide glutathione. **M.J. Panzner***, D. Hohman,
E. Elmond, M. Gehring, T.C. Leeper,
W. Youngs

11:55 Morning Closing Remarks

* Principle Author

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Hawaii Convention Center
Halls I, II, III

Inorganic Complexes for Solar Energy Harvesting (#256)

Organized by: M. Wolf, K. Sakai,
F. MacDonnell

Poster Session
10:00 – 12:00

1587. Synthesis and characterization of heteroleptic copper(II) complexes for light harvesting applications. **J. Huynh**,
B.D. Koivisto*

1588. Luminescent building blocks for supramolecules from a *bis*-diimine platinum(II) dithiolene with exchangeable diimine ligands. **B.W. Smucker***, J.B. Smith,
P.J. Derry

1589. Fabrication and properties of zinc oxide-based perovskite solar cells. **M. Fujibayashi**, h. morikawa, E. Inami,
H. Ogata

1590. Liquid light guides for photochemistry and photocatalytic experiments. **K. Nomura***, K. Hosoda, Y. Toyoda,
D. Yokota, Y. Morito, A. Fujishima

1591. Effects of silver nanoparticle addition to perovskite-based solar cells. **h. morikawa**, M. Fujibayashi, E. Inami,
H. Ogata

1592. High haze TCO glass to enhance the light harvest for dye-sensitized solar cell. **T. Endo***, R. Otsuka, R. Murakami,
M. Okuya

1593. Reduction of TiO_2 / TCO interface resistance for dye-sensitized solar cell with TNO transparent conductive film. **T. Endo***, M. Okuya, R. Iwaki,
S. Takemura, S. Nakao, S. Okazaki,
E. Sakai, N. Yamada, T. Hitosugi,
T. Hasegawa

1594. Molecular orientation control in phthalocyanine-based thin films using magnetic field. **Y. Fujita**, Y. Kitakuni,
A. Maeda*, K. Uemura, Y. Hirai

1595. Photohydrogen-evolving molecular device sacrificing initially collected one electron. **K. Yamamoto**, K. Kitamoto,
K. Sakai*

1596. Water soluble copper phthalocyanine as photochemical water oxidation catalyst. **R. Terao**, T. Nakazono, A.R. Parent,
K. Sakai*

1597. Iridium complexes with Coumarin ligands: Effective sensitizers for visible-light-driven hydrogen generation. **S. Takizawa***, S. Murata

1598. Syntheses and hydrogen-evolving activities of nickel(II) pyridinethiolate complexes stabilized oligopeptide moieties. **K. Miyazaki**, K. Kitamoto, K. Yamauchi,
K. Sakai*

1599. Dye-sensitized solar cells consisting of hierarchical thin-layered nanocrystalline TiO_2 . Pt nanoparticles from organic syntheses, and organic dyes of donor- π -acceptor type. **K. Mitsuke***, N. Tanaka,
A. Saito, D. Izutsu, K. Takahashi,
M. Wakayama, M. Hashimoto

1600. Encapsulation of Pt(II)-based molecular catalysts into a supramolecular cage and their catalytic activity for hydrogen evolution from water. **S. Tanaka**,
T. Nakazono, K. Yamauchi, K. Sakai*

1601. Ruthenium complex as a single-component redox shuttle for electrochemical photovoltaics. **J. Kim**, N. Jeong*

1602. Molecular catalysis of hydrogen evolution based on a one-step two-electron reduction scheme. **S. Nakashima**,

K. Yamauchi*, K. Sakai*

1603. Bis-Ru(II) complexes bearing a sulfur bridge of varying oxidation states for application in solar cells and light-emitting devices. **C.M. Brown***, M.O. Wolf

1604. Studies on electrochemical water reduction catalyzed by bis(dithiolato)nickelate(II) complexes. **K. Koshiba**,
K. Yamauchi*, M. Huynh,
S. Hammes-Schiffer, K. Sakai*

1605. Polypyridyl ruthenium(II) complexes in ion exchange resins toward solid-state light harvesting system. **A. Ito***, K. Kato,
N. Kishida, Y. Teki

1606. Photoinduced water oxidation properties of cobalt porphyrin catalysts. **T. Nakazono**, A.R. Parent, K. Sakai*

1607. Novel methods for catalyst functionalization of semiconductors and applications in photoelectrocatalysis. **S.C. Eady***, B. Brown, S. Peczonczyk,
S. Maldonado, N. Lehnert

1608. Pigment-acceptor-catalyst triads for photochemical hydrogen production from water. **K. Kitamoto**, K. Sakai*

1609. Dye-sensitized solar cells using cyclo-metallated ruthenium complexes and cobalt redox electrolyte. **T. Funaki***,
N. Onozawa-Komatsuzaki, K. Sayama

1610. Structure-activity relationship of photochemical H_2 evolution from water catalyzed by cobalt-NHC complexes. **K. Kawano**, K. Yamauchi*, K. Sakai*

Hawaii Convention Center
Halls I, II, III

Metal Mediated Polymerization (#292)

Organized by: P. Hayes, R. Waterman,
T. Mizuta, Y. Tang, S. Sangnirutnugul

Poster Session

10:00 – 12:00

1611. Cobalt amine-bis(phenolate) complexes for the activation of carbon dioxide. **K. Ambrose**, C.M. Kozak*

1612. Synthesis of polyolefin brushes by polymerization of α -olefins containing long branches. **S. Pengoubol**, K. NOMURA*

1613. New earth-abundant metal salen complexes for the copolymerization of carbon dioxide with epoxides. **H. Plommer**,
F. Kerton*

1614. Cr(III) amine-bis(phenolate) complexes as catalysts for the production of copolymers from CO_2 , epoxides, and lactide. **K. Ni***

1615. Preparation of pentacoordinate titanium *n*-butoxide derivatives, and their analysis by density functional theory calculations and nuclear magnetic resonance analysis. **K. Koike**

1616. Transition metal facilitated synthesis of nucleosidic polymers. **C.M. Mikulski***

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

S-block Metal Chemistry (#304)

Organized by: K. Ruhlandt-Senge,
P. Andrews, C. Cui

Presiding: P. Andrews, K. Henderson

8:00 – 1617. Molecular magnesium(II) compounds: Bespoke reagents for the synthesis of low-coordinate metal-metal bonded complexes. **C. Jones***

8:30 – 1618. Recent developments in the chemistry of compounds with Group 2-transition metal bonds. **P. Mountford***,
M.P. Blake

9:00 – 1619. Alkaline earth metal boronates: From structural studies to high resolution solid state NMR characterizations and computational modeling. **D. Laurencin***,
S. Sene, M. Reinholdt, C. Gervais,
D. Berthomieu, A. Mesbah, G. Renaudin,
M.E. Smith, c. bonhomme

9:20 – 1620. Ligation/solvation competition in heavy alkaline earth metal tetraaryborates. **K. Ruhlandt-Senge**, C. Lavin,
D. Allis, A. Goos, M. Gillett-Kunzath

9:40 – 1621. Addressing the limitations of s-block reactivity and catalysis. **M.S. Hill***

10:00 Break

10:10 – 1622. Aggregation and reactivity in organolithium reagents. **H.J. Reich**

10:40 – 1623. Group two mediated frustrated Lewis pairs: Meta-FLPs. **M.D. Anker***, M.s. Hill

11:00 – 1624. Chiral magnesium and calcium reagents in asymmetric deprotonation processes. **K. Henderson***

11:20 – 1625. Preparation and reactivity of soluble alkaline earth metal hydride complexes. **L. Fohlemeister**, A. Stasch*

11:40 – 1626. Trimagnesium complex of hexaaazatrinaphthylene trianion: A novel triradical with an open-shell doublet character. **J.O. Moilanen**, B.M. Day, T. Pugh,
R.A. Layfield*

Hawaii Convention Center
Halls I, II, III

Metal Coordination Sphere Design for Challenging Bond Transformations (#318)

Organized by: K. Caulton, A. Hill,
S. Johnson, M. Yamashita

Poster Session

10:00 – 12:00

1627. Search for active first-row transition metal alkylidene complexes. **A. Nielsen***,
J. Harrison, A. Sajjad, P. Schwertfeger

1628. Rigid 2,1,3-benzosiladiazole based PSi pincer ligands. **C. Ma**, A.F. Hill*,
L.S. Dixon, M. Sharma, A. Sinha,
J.S. Ward

1629. Pincer ligands with pyrazole arms: Redox-nonnucleophilicity expands chemical reactivity. **K. Caulton***

1630. Synthesis and reactivity of NHC-based rhodium macrocycles. **R.E. Andrew**,
D.W. Ferdani, C.A. Ohlin, A.B. Chaplin*

1631. Synthesis, structure, and property of Ir and Rh complexes bearing an P^{Pr} -substituted PBp ligand. **K. Tanoue**,
M. Yamashita

1632. Iridium catalyst featuring a hemilabile SINN-pincer ligand for Si-H deuteration of hydrosilanes with benzene- d_6 . **T. Komuro**, T. Osawa, R. Suzuki,
H. Tobita*

1633. Synthesis of first-row transition metal complexes with bis(aminomethyl)pyridine ligands and reactions of the iron complex involving β -hydrogen elimination. **T. Higashi**, T. Hatanaka, Y. Funahashi

1634. Enhanced catalysis – homo- and heterobimetallic complexes of Rh and Ir for C–X bond formation reactions. **M.B. Peterson***, S. Choy, M. Gatus,
B.A. Messerle

1635. Homoleptic Au(III) trications: A synthetic pathway to a new class of Au(III) compounds. **R. Corbo**, J.L. Dutton*

1636. Synthesis and reactivity studies of square pyramidal tantalum complexes. **G. Lavoie***, R. Morris

1637. Construction of multioffacial multinuclear complexes within a one-nanometer-size macrocyclic porphyrin nanoring. **Y. Ohkada***, A. Satake*

1638. Hemilabile pincer ligands for enhanced catalysis. **A. Gopalan Nair**

1639. Synthesis of early-late heterodinuclear complexes bearing ONO-P multidentate ligands. **S. Yoneyama**, K. Satou,
T. Hasegawa, N. Suzuki*, Y. Masuyama

1640. Photochemical reaction of diruthenium tetrahydride-bridged complexes with carbon dioxide: Insertion of CO_2 into a Ru-H bond vs. C=O double bond cleavage. **R. Shimogawa**, T. Takao*, H. Suzuki

1641. Perimidinylene based N-heterocyclic carbene pincer ligands. **C. Ma**,
A.F. Hill*, C.M. McQueen, J.S. Ward,
B.A. Messerle, M.J. Page

1642. Mechanistic investigation of H/D exchange of unactivated C–H bonds by a pentanuclear nickel cluster. **M.M. Shoshani**, S.A. Johnson*

1643. Synthesis of O, N – O, N – N ligands and their heterodinuclear complexes. **T. Shimamura**, K. Haraga, Y. Masuyama,
N. Suzuki*

1644. Non-innocent behavior of 3-coordinate phosphorus ligands: Late transition metal phosphido vs. phosphonium bonding and reactivity. **Y. Han**, A.F. Hill*,
Y. Xiong, T. Schwich

1645. Developing first-row transition metal catalysts that incorporate coordinatively versatile redox-active ligands. **C.E. MacBeth***, O. Villanueva

1646. Multidentate phosphine-enamide ligands for small molecule activation and catalysis. **V. Annibale**, T.G. Ostapowicz,
S. Westhues, C. Lenczyk, T.C. Wambach,
M. Fryzuk*

1647. New N-heterocyclic carbene ligands as supports for low valent metals: Synthesis and reactivity of first row NHC metal complexes. Z. Call,
A. Gaona-Rojas, C. Bradley*

1648. Synthesis and study of novel iron sulfide complexes as models for nitrogenase. **N.A. Arnet**, T.R. Dugan,
W.W. Brennessel, B.Q. Mercado, E. Bill,
P.L. Holland*

1649. Trigonal bipyramidal complexes with a stable copper(III) moiety and their oxygen-derivatives. **H. Chang**, W. Lee*

1650. Post functionalization: An effective method to construct heavier group 14 element donor-functionalized NHC complexes. **L. Deng***

1651. Ligand cooperation in the hydrogenation of N_2O using PCP iridium pincer complexes. **L.E. Doyle**, W.E. Piers*,
J. Borau-Garcia

1652. Phosphide-nickel(II) and phosphinite-nickel(0) interconversion via reversible P–O bond formation and cleavage. **S. Kim**, Y. Kim, S. Oh, Y. Lee*

1653. Transformation of (PEP)Ni-thiolate assisted by metal-ligand cooperation. **S. Oh**, Y. Lee*

1654. Copper-mediated cross-coupling reaction: mechanistic insights and its application. **M. Oi***, M. Otsuka, J. Kanazawa,
R. Takita, M. Uchiyama

1655. Synthesis and reactivity of electron rich amino-substituted diaryl PCP pincer complexes. **J.D. Smith**, S. Sugawara,
Y. Yamamoto, W.E. Piers*, D. Spasyuk

1656. Acceptoreless dehydrogenation of amines by cooperative $[\text{CpRu}(\text{P}^{\text{R}}_2\text{N}^{\text{R}}_2)_2(\text{NCMe})]^+$ complexes. **J.M. Stubbs***, J.M. Blacquiere

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NO Generation, Signaling and Reduction in Biological Systems (#371)

Organized by: N. Lehnert,
G. Richter-Addo, F. Doctorovich,
K. Fujisawa
Presiding: N. Lehnert

8:00 – 1657. Using biosynthetic models of nitric oxide reductase and nitrosocyanin to understand structures and mechanisms responsible for NO reduction and reversible S-nitrosylation. **Y. Lu***,
S. Chakraborty, S. Tian, J. Reed

8:30 – 1658. Molecular mechanism of NO reduction by bacterial nitric oxide reductases. **Y. Shiro**, T. Toshia, T. Kimura,
M. Kubo

9:00 – 1659. Using isotopic fractionation to provide insight into the mechanism of microbial N_2O production. **E.L. Hegg***,
H. Yang, H. Gandhi, A. McQuarters,
N. Lehnert, N.E. Ostrom

9:20 – 1660. Exploring the nitric oxide dioxygenase activity of heme-thiolate enzymes. **D. Stuehr***

9:50 Break

10:00 – 1661. Bending and stretching in six-coordinate iron nitrosyls. **W.R. Scheidt***,
Q. Peng, J. Pavlik, J. Sage

10:20 – 1662. Reduction of NO to HNO by antioxidants (alcohols, thiols, amines, and others). **F. Doctorovich**

* Principle Author

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onlineprogram

10:40 – 1663. HNO/NO conversion mechanisms of Cu-based HNO probes with implications for Cu,Zn-SOD and metal-based HNO probe design. M. Michael, G. Pizzella, L. Yang, Y. Shi, T. Evangelou, D. Burke, **Y. Zhang***

11:00 – 1664. Modeling nitric oxide signaling chemistry at copper and zinc sites. **T.H. Warren***

11:30 – 1665. Chemistry of iron-sulfur clusters in nitric oxide signaling. **E. Kim***

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Activation of Small Molecules by Electropositive Metals Related to Chemical Energy Conversion (#380)

Organized by: D. Mindiola,
H. Kawaguchi, L. Schafer, K. Meyer,
A. Veige, M. Reynolds
Presiding: K. Meyer, D. Mindiola

8:00 opening remarks

8:05 – 1666. Elucidating the Inorganic Enamine Effect: Fast Wittig-like reactions and CO₂ deoxygenation across a metal-carbon triple bond. **A.S. Veige***, S.d. Gonsales, M.E. Pascualini, I. Ghiviriga, K.A. Abboud

8:25 – 1667. Bimetallic cleavage of aromatic C–H bonds by rare earth metal complexes. **P.L. Diaconescu**

8:45 – 1668. Activation of strong bonds with low-valent Group 5 complexes. **J. Arnold**

9:05 – 1669. Scandium terminal imido complexes: Synthesis, structure, and reactivity. E. Lu, J. Chu, X. Han, **Y. Chen**

9:25 – 1670. Early metal catalyzed hydrodegradation of oxygenates. **A.D. Sadow***

9:45 – 1671. Early transition metal catalyzed C–H alkylation: Hydroaminoalkylation for the selective synthesis of amines. **L.L. Schafer***

10:05 break

10:20 – 1672. Early transition metal-catalyzed activation of $\alpha\text{-C}(\text{sp}^3)\text{-H}$ bonds of primary or secondary amines. **S. Doye***

10:40 – 1673. Metal-metal bonded catalysts for dinitrogen silylation and olefin hydrogenation. **C. Lu***, R. Siedschlag, L. Clouston, R. Cammarota, L. Gagliardi, E. Bill

11:00 – 1674. Transformation on titanium by reversible carbon–carbon bond cleavage. **T. Takahashi**

11:20 – 1675. Synthesis and reaction chemistry of (imido)vanadium(V)-alkyl, alkylidene complexes. **K. NOMURA**

11:40 – 1676. C–H and C–P activation and dehydrogenation reactions of alkanes with phosphino-alkylidene and -alkylidyne complexes of titanium. **D. Mindiola***

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

New Directions for Sensing Metals in Biology (#424)

Organized by: E. New, E. Que,
T. Hirayama
Presiding: E. Que

8:00 – 1677. Genetically encoded sensors for monitoring the spatial distribution of zinc in living cells. **A.E. Palmer**

8:30 – 1678. Development of genetically encoded zinc(II) and iron(II) biosensors to probe cellular metal homeostasis. **C.A. Fierke***, R.B. Thompson, B. Kim, C.A. Pitcairn, A.K. Stoddard, E.G. Matveeva

9:00 – 1679. Imaging properties of the (zinc)-proteome with zinc fluorophores. **D.H. Petering***, K. Fatima, M. Karim, E. Lund, M. Namdarghanbari, A. Nowakowski

9:20 – 1680. Methods for the fluorescent detection of heavy metals. C. Shen, D.G. Smith, **E. New**

9:40 – 1681. Strategies to develop whole-cell biosensors for heavy metals. **J. Zhao***, W. Wei

10:00 Morning tea

10:40 – 1682. Visualising ion flux with small molecule probes, nanoparticles and smartphones. **P. Rutledge***

11:10 – 1683. Illuminating reductase activity in hypoxia with chemiluminescent probes. **A.R. Lippert**

11:40 – 1684. Responsive probes based on luminescent iridium complexes. **F. Kielar**

Saturday Afternoon

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson,
G. Schreckenbach, T. Yaita, J. Li,
P. Yang
Presiding: R.J. Abergel, N. Kaltsosannis

13:00 – 1685. Synthesis and crystal structures of uranium, neptunium, and plutonium complexes of 2,2'-biphenylenedithiophosphinate and its "untethered" analog diphenyldithiophosphinate.

J. Macor, J.L. McDonald, J.N. Cross, S.R. Daly, A.J. Gaunt*, **G.S. Girolami***, M.T. Janicke, S.A. Kozimor*, M.P. Neu, S.D. Reilly, A.C. Olson, B.L. Scott

13:20 – 1686. Nanoscopic analysis of oxygen vacancy in nuclear oxide fuel.

K. Konashi*, T. Yato, M. Kato, M. Watanabe, T. Yaita, H. Shiwaku

13:50 – 1687. Accessing properties of large actinide systems with frozen-density embedding. **V. Vallet**, M. Olejniczak, F. Réal, A. Severo Pereira Gomes

14:20 – 1688. Achieving actinide and lanthanide group separation with hard–soft donor combined ligands. **W. Shi***, C. Xiao, Z. Chai

14:50 Break

15:05 – 1689. Experimental and theoretical investigations of metal–oxygen multiple bonding in actinyl ions. **S.G. Minasian**, E.R. Batista, C.H. Booth, J.M. Keith, W. Lukens, S.A. Kozimor, R.L. Martin, D.K. Shuh, X. Wen

15:25 – 1690. Spectroscopic and theoretical studies of gas phase actinide species. **M.C. Heaven**, J.H. Bartlett, R.A. VanGundy, K. Mascitolo

15:55 – 1691. X-ray spectroscopic studies of actinide-ligand interactions. **M.A. Denecke***

16:25 – 1692. Computational studies of the hydrolysis reactions of actinide ions and of novel bonding interactions for actinides. **D.A. Dixon**

16:55 – 1693. Correlated electronic states in actinide-based intermetallic compounds. **Y. Haga***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

Metal-Organic Frameworks: Synthesis, Properties and Applications (#50)

Organized by: G. Shimizu, J. Long,
M. Suh, Q. Xu, X. Chen

13:30 – 1694. Chemistry and application of soft porous coordination polymers. **S. Kitagawa***

14:00 – 1695. Phosphine coordination materials with defined open metal sites.

S.M. Humphrey*, J. He, A.M. Bohnsack, N. Waggoner, A. Nguyen, V.M. Lynch, J.E. Reynolds, S. Dunning

14:20 – 1696. Effect of ligand substitution on breathing mode of MOFs with MIL-53 type crystal structure. T. Ahnfeldt, M. Enssle, M. del Prado Carrion Ramirez, H. Fjellvåg, **P.D. Dietzel***

14:40 – 1697. Understanding metal-organic framework chemical stability properties via simulation and experiment. **K.S. Walton***, N.C. Burtch

15:00 – 1698. Gas separations in metal-organic frameworks. T.M. McDonald, E.D. Bloch, J.A. Mason, Z.R. Herm, B.M. Wiers, M.T. Kaplewski, M.I. Gonzalez, J.E. Bachman, D. Gygi, W.L. Queen, **J.R. Long***

15:30 – 1699. Chromatographic enantioseparation using double-pillared homochiral MOF in HPLC. **K. Tanaka***

15:45 – 1700. Nanospace within metal-organic frameworks: Plenty of opportunities for heterogeneous catalysis. **S. Ma***

16:05 – 1701. Single crystalline hollow metal-organic frameworks: A metal-organic polyhedron single crystal as a sacrificial template. **M. Lah***

16:25 – 1702. How to make conducting metal-organic frameworks. **T. Komatsu***, J.M. Taylor, T. Suguri, H. Kitagawa

16:40 – 1703. Tuning the photoredox properties of porphyrinic metal-organic frameworks for photocatalytic organic synthesis. **Z. Zhang**

16:55 – 1704. Isolation and studies of reactive heme species in metal-organic frameworks. J. Anderson, A. Gallagher, **D. Harris**

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62)

Organized by: H. Kageyama,
B. Kennedy, J. Wiley
Presiding: J.B. Wiley, H. Xiang, Z. Ye

13:00 – 1705. Strong carrier localization in LaVO₃-N_x perovskite-type oxynitride epitaxial thin films grown by nitrogen-plasma-assisted pulsed laser deposition.

M. Sano, Y. Hirose, S. Nakao, T. Fukumura, T. Hasegawa*

13:15 – 1706. Topotactic fluorination of perovskite-type strontium ruthenate thin films using polyvinylidene fluoride.

K. Kawahara*, A. Chikamatsu, T. Katayama, T. Onozuka, T. Fukumura, T. Hasegawa

13:30 – 1707. Bonding and electronic structures of electropositive metal germanides prepared by high-pressure synthesis containing germanium with unusual coordination numbers. **H. Fukukawa***, K. Baba, M. Yoshikawa, F. Ohtsu, D. Saito

13:50 – 1708. Novel low-dimensional magnets prepared by hydro(solvo)thermal method. **H. Lu**, H. Kageyama

14:10 – 1709. White-light emission from layered hybrid perovskites. E. Dohner, A. Jaffe, **K. Karunadasa**

14:45 – 1710. Accidental organic substitution in methylammonium lead perovskites. **J. McLeod***, L. Liu, S. Duhm, B. Sun, P. Shen, R. Wang, W. Xu

15:05 – 1711. Understanding the stability of materials for nuclear waste sequestration applications. E. Aluri, R. Rafiuddin, **A.P. Grosvenor***

15:25 – 1712. Role of noncovalent interactions in templated vanadates. **A. Norquist**

15:45 – 1713. Factors influencing framework structures and macroscopic centricities in mixed metal oxide materials containing local asymmetric units. **K. Ok***, D. Lee, Y. Kim, S. Bae, S. Bang, Y. Kim, H. Kim, S. Song, H. Jo

16:20 – 1714. Atom-by-atom synthesis of catalytic inorganic clusters within mesoporous metal-organic framework materials. **J. Hupp***

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications (#87)

Organized by: T. Storr, C. Grapperhaus, H. Fujii
Presiding: H. Fujii, T. Storr

13:00 – 1715. Redox-active metal-thiolates: Ligand-centered electrocatalytic proton reduction/hydrogen oxidation.

C.A. Grapperhaus, A.Z. Haddad, R. Jain, M. Mashuta

13:30 – 1716. Direct ligand-centered dehydrogenations by metal bis-iminosemiquinonates. **S.N. Brown***

14:00 – 1717. Aluminum-ligand cooperation in proton and electron transfer reactions. **L.A. Berben***, E.J. Thompson, T.J. Sherbow

14:30 – 1718. Molecular electrocatalysts bearing redox-active ligands for proton and carbon dioxide reduction: Synergy between experiment and theory.

J. Panetier*

14:50 Break

15:00 – 1719. Redox chemistry of coordinated anilines. **F. Thomas***, O. Jarayies, N. Leconte, C. Philouze, A. Kochem

15:30 – 1720. Investigating the electronic structures and reactivity of f-block elements bearing redox-active ligands. **S.C. Bart***

16:00 – 1721. Diiminepyridine titanium complexes. N. Rahimi, **P.H. Budzelaar***

16:30 – 1722. Molecular mechanism of heme axial ligand for controlling the reactivity of oxoiron(IV) porphyrin π-cation radical complex. **H. Fujii**

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Chemistry and Application of Boron Clusters (#152)

Organized by: S. Kang, N. Hosmane, D. Schubert, H. Nakamura, Z. Xie
Presiding: H. Nakamura

13:00 – 1723. Transition metal catalyzed functionalization of carboranes via B-H activation. **Z. Xie**

13:30 – 1724. Simpler route to polychlorinated monocarba-*cis*-dodecaborate and ammonio-*cis*-dodecaborate anions for use as weakly coordinating anions. **R.J. Wehmhschulte***, M. Saleh, D. Powell

13:50 – 1725. Charged carboranyl phosphine and carbene ligands in catalysis. **V. Lavallo***

14:20 Break

14:30 – 1726. LiCB₁₁Me₁₂ as a catalyst. P. Dron, Y. Hervault, T. Magnera, J. Kaleta, V. Volkis, K. Whittener, C. Little, **J. Michl***

15:00 – 1727. Inorganic boron clusters for solar energy harvest. Y. Cho, S. Kim, **H. Son***

15:20 – 1728. Inert B–H activation by metal–metal cooperativity. **H. Yan***

15:50 Break

16:00 – 1729. Cage molecule self-assembly. **P.S. Weiss***

16:30 – 1730. Boron oxide cluster chemistry of industrial borates. **D.M. Schubert***

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Current Trends and Interconnectivities Among Fundamental and Applied Inorganic Fluorine Chemistry (#156)

Organized by: K. Matsumoto, R. Hagiwara, G. Schrobilgen, H. Mercier, R. Syvert
Presiding: R. Syvert

*** Principle Author**

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13:00 – 1731. Stereochemical activity of the xenon electron lone pairs of $\text{F}_2\text{XeNCCH}_3$ and $\text{F}_2\text{Xe}(\text{NCCH}_3)_2$ – and the first of oxide and neutral oxide fluoride of Xe(I), $[\text{Xe}-\text{OxeOxe}]^{2+}$, and $\text{O}(\text{Xe})_2$.

G.J. Schrobilgen*, J. Haner,
M.V. Ivanova, K. Matsumoto,
H.P. Mercier

13:30 – 1732. Bromine-oxygen-(fluorine) compounds. **K. Seppelt***

14:00 – 1733. Novel high oxidized metal compounds. **S. Riedel***

14:30 – 1734. Xenon(VI) and xenon(VIII) oxide and oxide fluoride chemistry.

J.T. Goettel, H.P. Mercier,
G.J. Schrobilgen*

14:50 Break

15:05 – 1735. Inorganic and organic fluorine chemistry unit to advance pentafluorosulfanyl-(SF_5)-substituent chemistry.

A.V. Matsnev, S.P. Belina, S. Qing,
K.A. Berger, A.R. Scavuzzo, P. Dudzinski,
A. Dreier, G. Haufe, **J.S. Thrasher***

15:35 – 1736. Activation of SF_6 aromatics and SF_6 at palladium and rhodium complexes. **T. Braun***, C. Berg, L. Zamostna

16:05 – 1737. Structure of the discrete $\text{Al}_2\text{F}_9^{3-}$ and AlF_6^{2-} anions.

G. Veryasov*, F. Xu, K. Matsumoto,
R. Hagiwara

16:25 – 1738. Novel fluorous amphiphilic heteroleptic Ru-based complex for dye-sensitized solar cell: Excellent photostability, and hydrophobicity. **N. Lu***

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2

Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus, and Synthesis (#226)

Organized by: R. Waterman, F. Ozawa,
D. Gates, P. Leung
Presiding: J.D. Masuda

13:00 – 1739. Catalysis in service of main group chemistry: Metal-mediated and metal-free routes to molecules and materials based on elements from group 13–15. **I. Manners***

13:20 – 1740. Electrochromic conjugated organophosphorus materials. **T. Baumgartner**

13:40 – 1741. Novel transformations of polyphosphorus compounds. **M. Scheer**, A. Seitz, M. Eckhardt,
S. Heinl, C. Heindl

14:00 – 1742. Phosphonated-based materials: From the synthesis of innovative (co-)polymers to their applications. **S. MONGE**

14:20 – 1743. Advances in luminescent materials containing multiply bonded phosphorus. **J. Protasiewicz**

14:40 – 1744. Hexacoordinated phosphorus(V) anions: Synthesis, characterization, and application for cationic polymerization studies. **K. Hazin***, P. Siu, D.P. Gates

15:00 – 1745. Phosphole-based organic materials: Synthesis and applications to organic solar cells. **Y. Matano***

15:20 – 1746. Phosphorus recovery from iron-enhanced primary wastewater sludge. **R. Li***, X. Li, H. Li, J. Xu, L. LIN, Y. LI

15:40 – 1747. Sterically crowded triarylphosphines and their material oriented derivatives. **S. Sasak***, N. Morita, M. Yoshifumi

16:00 – 1748. Investigating the aromaticity in boron-phosphorus heterocycles. J. Barnard, **C.D. Martin**

16:20 – 1749. Toward new main group radicals and cations featuring phosphorus, carbon, and aluminum centers. **J.D. Masuda***

16:40 – 1750. Versatile reagent $\text{Ph}_3\text{As}(\text{OTf})_2$: One-pot synthesis of $[\text{P}_7(\text{AsPh}_3)_3]\text{[OTf]}_3$ from PCl_3 . **M. Donath***, J.J. Weigand

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

The Expanding Periodic Table: New Discoveries and Chemistry of the Heaviest Elements (#234)

Organized by: Y. Nagame, H. Nitsche,
Z. Qin, P. Schwerdtfeger, C. Duellmann,
A. Tuerler
Presiding: Y. Nagame, z. qin

13:00 – 1751. First synthesis and investigation of $\text{Sg}(\text{CO})_6$. **J. Even***

13:30 – 1752. Formation and gas phase chemistry the transition metal carbonyl complex. **z. qin***

14:00 – 1753. Theoretical studies of the electronic structures of seaborgium carbonyls $\text{Sg}(\text{CO})_n$ ($n = 1 – 6$). **W. Xu, J. Li***

14:30 – 1754. Recent progress in theoretical predictions of chemical properties of the heaviest elements. **V. Pershina***

15:00 – 1755. Chemistry of element 114, fermium. **A. Yakushev***

15:30 – 1756. Gas phase chemical investigation of element 113 and beyond. **R. Eichler***

16:00 – 1757. Present status and future plans of chemical experiments with superheavy elements at PSI/UNIBE. **A. Türler***

16:30 – 1758. Development of a rapid solvent extraction apparatus for aqueous chemistry of the heaviest elements. **Y. Komori***, H. Haba, K. Ooe,
A. Toyoshima

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Advances in the Medicinal Applications of N-Heterocyclic Carbene Metal Complexes and Azolium Cations (#255)

Organized by: W. Youngs, M. Baker,
C. Che, I. Lin, M. Panzner

13:00 Opening Remarks

13:10 – 1759. New classes of Au-NHC complexes as potential anticancer agents. **M. Baker***, J. Hickey, A. Magee,
B.W. Skelton, W. Zhao

13:45 – 1760. Gold complexes of N-heterocyclic carbene ligands: Luminescent probes and anticancer properties. **C. Che**

14:20 – 1761. Heterometallic titanium-gold and ruthenium-gold carbene complexes with potential as cancer chemotherapeutics. **M. Contel***, J. Fernandez-Gallardo,
V. Mui, B. Elie, R. Collison

14:55 Break

15:10 – 1762. Development of imidazolium salts for cancer therapy. **W. Youngs***,
P.O. Wagers, K.L. Shelton, M.A. DeBord,
M. Southerland, M.J. Panzner,

A. Tarabolti, C.A. Tessier, L.P. Shriner

15:45 – 1763. Kinetic studies of n-heterocyclic carbene ruthenium complex as self-regenerative antioxidant. **Y. Htet***,
A.G. Tennyson

16:20 Closing Remarks

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

S-block Metal Chemistry (#304)

Organized by: K. Ruhlandt-Senge,
P. Andrews, C. Cui
Presiding: K. Ruhlandt-Senge

13:00 – 1764. Amazing world of functionalized organolithium compounds: New synthetic tactics and strategies, mechanistic and structural insights. **V. Capriati***

13:30 – 1765. Flash chemistry using short-lived organolithium species. **J. Yoshida***

14:00 – 1766. Allylphosphine reactivity: De-protonation vs. P-C bond cleavage synthetic and DFT calculation studies. **V.L. Blair***, C. Thompson

14:20 – 1767. Remarkable homoleptic thioether and phosphine coordination to s-block cations. M. Champion,
M. Caravetta, J. Dyke, W. Levason,
D. Pugh, **G. Reid***, W. Zhang

14:50 Break

15:00 – 1768. S-block syntheses sans solvent: mechanochemical insights into organometallic reactions. N. Rightmire,
T.P. Hanusa*

15:30 – 1769. Novel reactivities of carbonoids towards E-H bonds. **S. Molitor***,
V.H. Gessner

15:50 – 1770. Steric hindrance matters.

P.G. Williard*, C. Su, J. Guang,
R. Hopson, Q.P. Liu, W. Li, G. Kagan,
C. Liu

16:20 – 1771. Synthetic applications of lithium amides and lithium enolates.

S.D. Bull

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Metal Coordination Sphere Design for Challenging Bond Transformations (#318)

Organized by: K. Caulton, A. Hill,
S. Johnson, M. Yamashita
Presiding: L. Deng, B.A. Messerle

13:00 – 1772. Iron catalysts with carboxyl-amido ligands for regio-selective hydroxylation. **Y. Hitomi**

13:20 – 1773. Potent reactivity in solubilised oxo-titanium polymers. **A. Nielsen***,
J. Waters

13:40 – 1774. Chelate-assisted B–H, Si–H and C–H activation for the installation of unconventional pincer ligands. **A.F. Hill***

14:00 – 1775. Main group elements in very low oxidation states stabilized by diimino-pyridine ligand. **T. Chu, G. Nikonor***

14:15 – 1776. Disilafuracycle complexes containing weakly coordinated η^2 -(H-Si) ligands. **Y. Sunada***, H. Tsutsumi,
H. Soejima, H. Nagashima

14:30 – 1777. Coordination chemistry of low-valent nickel pincer complexes. **Y. Lee***

14:45 – 1778. Planar chiral platinum metal complexes of phosphonium-1-indenylides. **M.C. Baird***, K. Purdaiva ,
K.G. Fowler

15:05 – 1779. Why cyclooctane metathesis does not give polyethylene with single site W based catalysts? **J. Bassett***,
M. Samantaray, E. Callens, N. Riache,
R. Dey, A. Hamielec, N. Kharbatia

15:25 – 1780. Magnesium amidinates and related compounds for catalytic bond formation. **M.P. Coles**, R.J. Schwamm,
B.M. Day, N. Mansfield, W. Knowelden,
C.M. Fitchett, P. Hitchcock

15:45 – 1781. Facile C–H metathesis of nitriles under mild conditions and subsequent catalytic C–C bond formations.

M.G. Gardiner*

16:00 – 1782. Bidentate nitrogen chelated Rh(I) complexes for CH activation and functionalization. **M. Webster-Gardiner***,
B. Vaughan, R. Fu, P. Piszel, R. Nielsen,
W. Doddard III, T. Cundari, T.B. Gunnoe

16:15 – 1783. Regioselective carbon-fluorine bond activation of perfluoroalkene on palladium(0). **M. Ohashi***, M. Shibata,
H. Saito, S. Ogoshi*

16:30 – 1784. In situ – formation of neutral rhodium(I) complexes and systematic investigations – application of the results.

H. Drexler, A. Meissner, S. Wei, B. Breit,
D. Heller*

16:45 – 1785. Ligand reactivity of (PNN)Rh complexes. **B. de Bruin***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

The Bio-Coordination Chemistry of Nitric Oxide and its Derivatives: Mechanisms of NOx Generation, Signaling and Reduction in Biological Systems (#371)

Organized by: N. Lehnert,
G. Richter-Addo, F. Doctorovich,
K. Fujisawa
Presiding: G.B. Richter-Addo

13:00 – 1786. NO and N_2O binding, activation and reduction by Fe and Cu active sites. **E.I. Solomon***

13:30 – 1787. Reactivity of a three-coordinate nickel nitrosyl cation. **A.M. Wright**,
T. Hayton

14:00 – 1788. Advanced thromboresistant/bactericidal nitric oxide releasing materials/devices for biomedical applications.

M.E. Meyerhoff*, Y. Wo, E.J. Brisbois,
H. Ren, N. Lehnert, A.P. Hunt

14:20 – 1789. Subcellular localization and cytotoxicity efficiency of nitrosyl ruthe-nium derivatives as nitric oxide delivery agents. **R.S. da Silva***, t. Joli, L. Negri,
J. Fernandes, L. Maximo, J. Moraes

14:50 Break

15:00 – 1790. N- and S-speciation of products in reactions of GSNO and H_2S .

P.J. Farmer*, M.R. Kumar, T. Clover,
A. Olaitan, T. Solouki

15:20 – 1791. Transition-metal nitrosyl com-

plexes ligated by hindered hydrotris(pyrazolyl)borate ligands. **K. Fujisawa**

15:40 – 1792. Iron-nitrosyl models for Class III dioxygenases. **F.A. Chavez***, J. Li,
A. Banerjee, P. Pawlak, W.W. Brennessel

16:00 – 1793. Insights into nitric oxide scavenging by flavodiron proteins. N. Giri,
A. Weitz, J. Caranto, R.E. Frederick,
M. Hendrich, **D. Kurtz***

Hilton Hawaiian Village
Kalia Tower, Kahili 2

Activation of Small Molecules by Electropositive Metals Related to Chemical Energy Conversion (#380)

Organized by: D. Mindiola,
H. Kawaguchi, L. Schafer, K. Meyer,
A. Veige, M. Reynolds
Presiding: L.L. Schafer, A.S. Veige

13:00 opening remarks

13:05 – 1794. Activation of SO_2 with di- and trivalent lanthanide complexes.

P.W. Roesky*

13:25 – 1795. Activation of small molecule oxidants at low-valent uranium centers.

S.C. Bart*

13:45 – 1796. Splitting and functionalization of N_2 mediated by pincer complexes: Early vs. late transition metals.

S. Schneider

14:05 – 1797. Activation of platinum complexes by ligand-based reactions with Lewis acids. **T. Tilley**, R. Bergman,
A.L. Liberman-Martin

14:25 – 1798. Heterobimetallic and trimetallic complexes based on the redox-active cofactor $\text{M}(\text{SNS})_2$ ($\text{M} = \text{Cr}, \text{Mo}, \text{W}$).

A. Heyduk, K. Rosenkoetter, M. Wojnar

14:45 session break

15:00 – 1799. Mechanism of the 4-electron oxidative addition of O_2 . E. Akturk,
G.P. Yap, **K.H. Theopolis**

15:20 – 1800. Complex intermediacy of hydrazine in molybdenum-based dinitrogen reduction. B. Billow, S. DiFranco,
A. Odom*

15:40 – 1801. Small molecule activation by tantalum amido-phosphine complexes.

M. Fryzuk, K.D. Parker

16:00 – 1802. Dinitrogen activation by multi-nuclear titanium polyhydride complexes.

T. Shima, S. Hu, G. Luo, X. Kang, Y. Luo,
Z. Hou*

16:20 – 1803. Activation of CO_2 at reactive coordination complexes of uranium.

K. Meyer*

* Principle Author

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Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

New Directions for Sensing Metals in Biology (#424)

Organized by: E. New, E. Que,
T. Hirayama
Presiding: T. Hirayama

- 13:00 – 1804. Imaging copper by MRI – promises and compromises. **V. Pierre**
 13:30 – 1805. Highly sensitive MR molecular probes toward in vivo metal ion sensing. **H. Nonaka***
 14:00 – 1806. 19F MRI contrast agents for imaging metals and biological redox chemistry. **E. Que***
 14:20 Afternoon tea
 14:50 – 1807. Photodecarboxylation as an alternative to nitrobenzyl groups in the construction of photocaged complexes. **S.C. Burdette***, P. Basa, S. Antala , R. Dempski
 15:20 – 1808. Development of photoacoustic strategies for metal ion sensing in vivo. **J. Chan***
 15:40 – 1809. Targeting metalloenzymes without affecting metal ion distribution: A safer and more effective strategy for treating neurological disease?. **M. Bourassa***, S. Karrupagounder, R. Ratan
 16:00 – 1810. Metal ion sensing using phosphorothioate modified DNAszymes. **J. Liu**
 16:20 – 1811. Molecular probes for the study of metal homeostasis: Fluorescent indicators and beyond. Q. Lin, B. Pinto-Pacheco, J. Pitteloud, S.C. Schwartz, **D. Buccella***

Saturday Evening

Hawaii Convention Center
Halls I, II, III

Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson, G. Schreckenbach, T. Yaita, J. Li, P. Yang

Poster Session
19:00 – 21:00

1812. Electrochemical properties of ruthenium complexes bearing multipod pyrene anchors on nanocarbon materials toward application of energy storage devices. **M. Kohmoto**, H. Ozawa, M. Haga
 1813. Developments of the collection apparatus for recoil products and spectrometer of low-energy internal-conversion electrons to study the deexcitation process of ^{235m}U . **Y. Shigekawa**, Y. Kasamatsu, A. Shinohara
 1814. Structural trends and property correlations in f-element chromates. **A.A. Arico***, T.E. Albrecht-Schmitt
 1815. Theoretical insights into the metal-metal multiple bonding in actinide dimetallic alcochenes. **C. Wang**, J. Lan, Q. Wu, Z. Chai, W. Shi*
 1816. Effect of substituents in 1,2,4-triazin-3-yl 1,10-phenanthroline on the extraction and complexation of Am^{3+} and lanthanide series elements. **A. Kamezawa***, S. Suzuki, T. Kobayashi, K. Sueki
 1817. SMM starting material U(III) preparation from aqueous salts. **T. Yamamuro***
 1818. $\text{Th}(\text{VO}_3)_2(\text{SeO}_3)$ and $\text{Ln}(\text{VO}_3)(\text{IO}_3)$ ($\text{Ln} = \text{Ce, Pr, Nd, Sm, and Eu}$): Unusual cases of alovalent substitution. **T.M. Eaton**, J. Lin, J.T. Stritzinger, T.E. Albrecht-Schmitt

Hawaii Convention Center
Halls I, II, III

Metal-Organic Frameworks: Synthesis, Properties and Applications (#50)

Organized by: G. Shimizu, J. Long, M. Suh, Q. Xu, X. Chen

Poster Session

19:00 – 21:00

1819. Effect of heat-treatment on catalytic activity of moisture-absorption MOF-5. **M. OKADA***, Y. Kitagawa, T. Sato, T. Hiaki
 1820. Metal-organic frameworks for device fabrication. **P. Falcaro**
 1821. Syntheses and physical properties of AgRh solid solution alloy nanoparticles coated with HKUST-1. **G. Li***, H. Kobayashi*, K. Kusada*, H. Kitagawa*
 1822. Synthesis of metal organic framework containing ferrocenium ion derivatives and their orientation control by magnetic field. **S. Tomoguchi***, S. Takaishi, H. Iguchi, K. Kagesawa, M. Yamashita
 1823. Hydrothermally stable metal-organic frameworks for Xe/Kr separation. M. Kim, **S. Lee***, T. Yoon, S. Kim, Y. Bae*
 1824. Enhanced physical properties of porphyrin based metal-organic frameworks by effective silica armoring. **Y. Kim***, Y. Kim, E. Choi*
 1825. Efficient separation of SF_6/N_2 mixtures using isostructural of metal-organic framework with proper pore sizes. **M. Kim***, S. Lee, S. Kim, A. Kim, Y. Bae*
 1826. Stability evaluation of microporous zeolitic imidazolate frameworks in dynamic atmospheres. **C. Mottillo**, T. Friscic
 1827. Electric conductive Hofmann-type porous coordination polymers incorporated Creutz-Taube-type complex module. **A. Mishina**, W. Kosaka, H. Miyasaka, T. Koshiyama, M. Ohba*
 1828. Development of a new crystalline sponge with structural flexibility and molecular recognition. **K. Matsumura**, T. Arai, Y. Inokuma, M. Fujita*
 1829. Synthesis, crystal structure, and physical properties of a novel metal-organic framework based on networked coordination nickel square motif. **R. Hashiguchi***, K. Otsubo, H. Kitagawa
 1830. Fabrication of nanoscale thin film using porphyrin-based SURMOFs concept. **S. Laakroekkiet**, M. Hara, S. Nagano, Y. Nagao*
 1831. Ionic liquid-modified microenvironment of nanocage of ZIF-8: Improvement of the molecular sieving properties. **Y. Ban, Y. Li, W. Yang**
 1832. Metal-organic frameworks with ferrocenedicarboxylic acid as building block. **A. Reiber***
 1833. Synthesis, structural characterization, and photoluminescent property of two Ho(III)-square (C₄O₄²⁻) coordination polymers. **C. Wang**
 1834. Effect of cation and anion of ionic liquid in ionothermal synthesis of Co-BTC meta-organic framework. **C. Han***, Y. Jung, E. Choi*, Y. Cha
 1835. Coordination-driven self-assembly of water soluble rectangles incorporating Ru(II) p-cymene acceptors and pyridyl donors with hydrophilic chains. **N. Singh***, Y. Song, D. Kim, T. Kim, K. Chi*
 1836. Thin film deposition of metal-organic frameworks(MOFs) on functionalized self-assembled-monolayer(SAMs). **Y. Jung***, J. Kweon, C. Han, E. Choi*
 1837. Electric responses on gas adsorption processes in a porous paddlewheel-type ruthenium dimer chain compounds. **W. Kosaka***, J. Zhang, Y. Sekine, K. Taniguchi, H. Miyasaka
 1838. Studies on the formation process of coordination polymers for photoluminescent material. **K. Kakutaka**, K. Nishikawa, Y. Morimoto, Y. Tachi*
 1839. Electric conductive property of Hofmann-type coordination polymers including Pt-I chain pillars. **S. Shimoda***, A. Mishina, W. Kosaka, H. Miyasaka, T. Koshiyama, M. Ohba
 1840. Layered phenylbutyl-methyl zirconium phosphonates: A novel archetype of a layered material that combines both stepwise and gradual d-spacing changes as stoichiometric ratio of pendant groups varies. **M.R. Manney, W.R. Leonstra***
 1841. Polyhedral oligomeric silsesquioxane functionalized metal-organic frameworks and their sorption properties. **Y. Hwang**, J. Chang
 1842. Synthesis and structural change of naphthalenediimide-based coordination polymers. **M. Miyata**, H. Iguchi*, S. Takaishi, M. Yamashita*
 1843. Creation of electrical conductive metal-organic frameworks. **T. Suguri***, K. Otsubo, H. Kitagawa
 1844. Construction and structural transformation of porous framework with coordinatively unsaturated sites by the self-assembly of discrete Rh(II) dimer units. **T. Itoh**, M. Kondo*, K. Wakabayashi, M. Kanaike, S. Masaoka*
 1845. Construction of metal organic framework-motor protein conjugates. **M. Ito***, T. Ishiwata, K. Kokado*, A. Kakugo, K. Sada
 1846. Rational design and synthesis of $\text{Ni}_{x}\text{Co}_{3-x}\text{O}_4$ nanoparticles derived from multivariate MOF-74 for supercapacitors. **M. Xue***
 1847. EPR spectroscopy of manganese-doped perovskite-type $[(\text{CH}_3)_2\text{NH}_2]\text{Zn}(\text{HCOO})_3$ metal-organic framework. **M. Simenas***, M. Maczka, A. Pöppel, J. Banyś
 1848. Theoretical investigation of interaction between gas molecules and Cu(II) open metal site in porous coordination polymer, and separation mechanism of CO over N_2 . **H. Hijikata***, S. Sakai
 1849. Preparation and catalytic properties of coordination polymer catalysts decorated with Pt nanoparticles. **S. Yoshimaru**, M. Sadakiyo, K. Kato, M. Yamauchi*
 1850. Engineering homochiral MOFs by spatially separating 1D chiral metal-peptide ladders: Tuning the pore size for enantioselective adsorption. **K.C. Stylianou***
 1851. New Hf-oxide based metal-organic frameworks with size selective gas adsorption properties. **R. Fujita***, Y. Kataoka, T. Kawamoto, M. Handa
 1852. Metal-organic frameworks: From rectangular to stellated and interpenetrating polyhedra. **M. Lahav***
 1853. Palladium detection and sorption by sulfur-laced MOFs: Implications for heterogeneous catalysis and nuclear wastes. **Z. Xu**
 1854. Salen metalloligands: Design strategy, catalytic ability, and functionality en route to their incorporation into metal-organic frameworks. **M. Solomon**, T. Church, K.A. Jolliffe, D.M. D'Alessandro*
 1855. Size-specific catalytic reactions based on immobilization of acids in metal-macrocyclic framework. **H. Yonezawa**, S. Tashiro, R. Kubota, T. Umeki, M. Shionoya
 1856. Investigation of electroactive and donor-acceptor metal-organic frameworks (MOFs) as tunable, functional materials. **C.F. Leong***, B. Chan, T.B. Faust, D.M. D'Alessandro
 1857. MOFs as supramolecular building blocks: Tuning aromatic-aromatic interactions in lamellar solids. **J.K. Klosterman***
 1858. Asymmetric construction of a ferrocenyl phosphapalladacycle from achiral enones and a demonstration of its catalytic potential. **K. Gan***, **S. Abdul**, C. Xu, Y. Li, S.A. Pullarkat
 1859. Assembly of hybrids based on polyoxotungstates and Co-tris(midazolyl) complexes with bifunctional electrocatalytic activities. **W. Zhou***, **J. Peng***, **Z. Zhang***
 1860. Guest responsive luminescent coordination polymers having a PTS-type framework. **H. Miura***, A. Mishima, T. Koshiyama, M. Ohba
 1861. Direct visualization of guest dynamic behaviors in ultramicroporous crystal for exceptional thermal expansion. **H. Zhou**, J. Zhang, X. Chen
 1862. Theoretical and experimental studies of H_2 , n_2 , CO and CO_2 adsorption of porphyrin based metal-organic framework. **Y. Kim***, Y. Kim, Y. Jung, C. Han, I. Kim, E. Choi*
 1863. Metal-organic framework as platform to tune the magnetization dynamics of single-molecule magnet. **W. Shi***, P. Cheng
 1864. Photofunctional zwitterionic metal-organic frameworks with tunable adsorption properties. **M. Wriedt**, D. Aulakh, W. An, H. Bilan
 1865. Two-legged mixed-valence metal-organic ladder compounds with mechanically interlocked molecules. **K. Otsubo***, K. Sugimoto, H. Kitagawa
 1866. Significant enhancement of hydrogen-storage capacity and speed in metal nanocrystals covered with a metal-organic framework. **H. Kobayashi***, G. Li, K. Kusada, H. Kitagawa
 1867. Microwave-assisted continuous synthesis of MOF-74(Ni) under moderate pressures. **G. Albuqueque**, R. Fitzmorris, M. Ahmadi, G. Herman*
 1868. Syntheses and physical properties of Ni and Pt nanoparticles covered with a metal-organic framework. **Y. Aoyama***, H. Kobayashi, M. Maesato, H. Kitagawa
 1869. Versatile topological MOFs built from substituted biphenyldicarboxylic acid. **J. Ma, T. Qin, X. Wang, D. Zhu***
 1870. Metal-organic frameworks-based materials for electrochemical sensing of carbon dioxide. **J. Kim, N. Jeong***
 1871. Synthesis of bifunctional $\text{NH}_2\text{-MIL}-101(\text{Cr})/\text{SiO}_2/\text{Fe}_2\text{O}_4$ magnetic catalysts and their catalytic performance of Knoevenagel reaction. **S. Ji**, S. Jiang, F. Habimana
 1872. Metal-organic graphene analogs based on hexathiolate linkers. **A. Tskhovrebov***, J.R. Long
 1873. Metallocopolycapsular networks based on a 1,3-alternate calix[4]arene derivative. **K. Park***, E. Lee, H. Ju, S. Moon
 1874. Stereoelectronic diversity for transition metal catalysis in metal organic frameworks. **R.G. Van Zeeeland**, X. Li, W. Huang*, L.M. Stanley*
 1875. Metal organic frameworks based on bulkiness building blocks for selective hydrogen adsorption. **B. Wu***, S. Takaiishi, M. Yamashita
 1876. Construction and luminescent property of a novel 3D metal-organic framework [Cd(pip)]. **Y. Zhang, H. Hu, X. Zhou, X. Zhang***
 1877. Heterometallic triazole MOFs for catalytic CO_2 transformation to cyclic carbonates. **D. Park***, R. Roshan, K. Bhin
 1878. Proton-conducting metal-organic frameworks: Molecular design and performance improvement. **.. Song, C. Hong**
 1879. Design and properties of new phosphonate monoester based metal-organic framework. **B.S. Gelfand**, J. Lin, G. Shimizu*
 1880. Development and structural transformation of porous framework constructed by multipoint arene-perfluorocarene ($\text{Ar}-\text{Ar}'^F$) interaction. **M. Kondo***, T. Itoh, S. Masaoka*
 1881. Synthesis and functional applications of aluminum metal-organic frameworks. **C. Lin**
 1882. Synthesis and structural comparison of 2D coordination polymers based on copper(II) and (S)-4,4'- and (S)-5,5'-Bis(4-carboxyphenyl)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl linkers. **W.W. Lestari***
 1883. Synthesis, structure and biological activity of dihydropyrimidinyl methanesulfonate complexes. **S. Huang***, J. Zhou*, D. Lu*, R. Yang*, **Y. Xie***

* Principle Author

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- 1884.** Post-synthetic copper metatlation of a Zr-based PCP with bipyridine units for heterogeneous selective oxidation.
K. Miyahara, T. Toyao, Y. Horuchi*, M. Matsuoka*
- 1885.** Series of cyanoacetato copper(II) coordination polymers with various *N,N'*-ditopic spacers: Structural diversity, supramolecular robustness, and magnetic properties. **J. Boonmak***, P. Suvanvapee, C. Pakawatchai, K. Murray, S. Youngme
- 1886.** Construction of photoactive frameworks with open metal sites. **P. Chinapang**, T. Itoh, M. Kondo, S. Masaoka*

Hawaii Convention Center
Halls I, II, III

From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62)

Organized by: H. Kageyama, B. Kennedy, J. Wiley

Poster Session
19:00 – 21:00

- 1887.** Preparation and magnetic properties of Y-type ferrite $\text{Ba}_2\text{Zn}_2\text{Fe}_{12}\text{O}_{22}$ substituted with Li and Al. **S. Ono**, M. Nakanishi, J. Kano, T. Fujii
- 1888.** High-pressure synthesis and ferroelectricity of A-site ordered double perovskite oxide $\text{Ca}^{\text{A}'}\text{Ti}_2\text{O}_6$ (A' : divalent cation). **Y. Akama**, D. Mori, Y. Inaguma*
- 1889.** Synthesis and properties of intermediate-temperature-type proton conductors with perovskite-related structures. **M. Saito**, T. Motohashi, H. Yamamura
- 1890.** Synthesis and magnetic properties of LaFeO_3 nanoparticles. **D. Takemura**, T. Fujii, J. Kano, M. Nakanishi
- 1891.** Crystal structures and magnetic properties of pseudo-1D molybdenum oxides $\text{Ln}_x\text{Mo}_2\text{O}_{12}$ ($\text{Ln} = \text{Y}, \text{Dy-Lu}$). **M. Miura***, M. Wakushima, Y. Hinatsu
- 1892.** Low temperature synthesis by ion exchange method and electrical conductivity of $\text{MgM}_{1-x}\text{V}_x\text{O}_3$ ($\text{M} = \text{Mn}, \text{Ti}, \text{Nb}, \text{Ta}, \text{Ru}, \text{Zr}$). **R. Hoshida**, D. Mori, Y. Inaguma*
- 1893.** Selective crystal growth and the impact of the local structure in $\text{Mn}_3\text{Tz}_2\text{O}_8$. **K. Rickert***, E.A. Pozzi, R. Khanal, G. Trimarchi, M. Onoue, J.E. Medvedeva, M.C. Hersam, R.P. Van Duyne, K.R. Poeppelmeier
- 1894.** Crystal structure and dielectric property of perovskite-type oxynitrides $\text{La}_{1-x}\text{Sr}_x\text{TiO}_{2+\gamma}\text{N}_{1-x}$. **D. Habu***, Y. Masubuchi*, I. Motohashi*, S. Kikkawa*

- 1895.** Li-filled double-deck layered structure of the $\text{RELi}_x\text{Cu}_{2-y}\text{P}_2$ ($\text{RE} = \text{La, Pr, Nd, Gd, Er}$; $0.82 \leq x \leq 1$; $1.19 \leq y \leq 1.54$) series: Experimental and theoretical studies. E. Jang, G. Nam, H. Woo, J. Lee, M. Han, S. Kim, **T. You***
- 1896.** Sintering of SrTa_2N oxynitride perovskite by using SrCN_2 sintering aid. **A. Hosono***, Y. Masubuchi*, T. Motohashi*, S. Kikkawa*

- 1897.** High-pressure synthesis, formation behavior, structure, and electronic conductivity of PbZn_3 with LiNbO_3 -type structure. **D. Mori**, K. Tanaka, Y. Inaguma*
- 1898.** Hydrogen ion beam irradiation effects on ZnO thin films studied by *in-situ* variable-temperature electrical resistivity measurements. **R. Nakayama***, M. Maesato, T. Nagaoka, M. Arita, H. Kitagawa

- 1899.** High-pressure synthesis and electrical properties of ternary electropositive metal germanides. **T. Nishikawa**, H. Fukuoka*, K. Inumaru
- 1900.** Synthesis and magnetic properties of electron- and hole-doped europium chalcogenides. **N. Rosa**, W.L. Boncher, S.L. Stoll

Hawaii Convention Center
Halls I, II, III

Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications (#87)

Organized by: T. Storr, C. Grapperhaus, H. Fujii
Presiding: H. Fujii, C.A. Grapperhaus, T. Storr

Poster Session
19:00 – 21:00

- 1901.** Unusual electronic structures in verdazyl coordination compounds. **D.J. Brook***, D. Chung, C. Fleming, B. Ploof, E. Johnson
- 1902.** Investigation of valence tautomerism in cobalt-dioxolene complexes using X-ray absorption and emission spectroscopy. **H.W. Liang**, D. Nordlund, T. Weng, D. Sokaras, C. Pierpont, K. Gaffney*
- 1903.** Synthesis, characterization, and catalysis of cobalt and molybdenum shvo-type catalyst. **W. Wu***, T. Seki*, D. Solis, R. Waymouth
- 1904.** Physicochemical properties of the oxidized forms of $\text{Pt}(\text{II})$ -dimine complexes with catecholate and benzenedithiolato. **S. Yamada**, M. Wakizaka, T. Matsumoto, H. Chang*
- 1905.** Crystal structure and property of dinuclear $\text{Co}(\text{III})$ complex with conjugated bis(catecholate) ligand. **Y. Suenaga***, K. Uwai
- 1906.** Electronic structure and reactivity of mono and bimetallic complexes containing redox active ligands. **R.M. Clarke**, J.R. Thompson, D. Savard, T. Storr*
- 1907.** Redox active ligands: Ligand-centered electrocatalytic proton reduction and hydrogen oxidation. **A.Z. Haddad***, R. Chauhan, C.A. Grapperhaus*
- 1908.** Interconversions of non-innocent-type and Schiff base nickel complexes acting as efficient water reduction catalysts. **S. Inoue***, Y. Kataoka, M. Handa, T. Kawamoto
- 1909.** Synthesis, characterization, and electrochemical properties of new tetra coordinated Ni (II) and Zn (II) complexes with new P_2S_2 type ligand framework. **R. Jain**, A.Z. Haddad, M. Mashata, C.A. Grapperhaus*
- 1910.** Redox chemistry of PCP-bridged chalcogen-centered ligands. **T. Chivers***, J. Konu, M. Risto, H.M. Tuononen

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Chemistry and Application of Boron Clusters (#152)

Organized by: S. Kang, N. Hosmane, D. Schubert, H. Nakamura, Z. Xie
Presiding: D.M. Schubert

- 19:00 – 1911.** Cellulose nanomaterials modified with carborane as sensors. **K.R. Carter***, K. Martin, J.J. Peterson
- 19:30 – 1912.** Cyclometalated iridium complexes with o-carboranes: Impact of o-carborane on the photophysical properties. Y. Lee, N.V. Nghia, M. Kim, M. Lee*
- 20:00 – 1913.** Design and applications of stimuli-responsive organoboron complexes with aggregation-induced emission properties. **K. Tanaka***, Y. Chijo*
- 20:30 – 1914.** Carborane photochemistry. Y. Cho, S. Kim, **S. Kang**

Hawaii Convention Center
Halls I, II, III

Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus, and Synthesis (#226)

Organized by: R. Waterman, F. Ozawa, D. Gates, P. Leung

Poster Session

19:00 – 21:00

- 1915.** Pd-catalyzed asymmetric Michael addition of diphenylphosphine. **X. Li**, R.J. Chew, P. Leung
- 1916.** Creation of phosphorus-boron bonded compounds featuring a pentavalent phosphorus atom. **N. Kano***, N.J. O'Brien
- 1917.** Metal carbonyl complexes of *N*-heterocyclic carbene-phosphinide adducts. **D. Bockfeld**, A. Doddi, P. Jones, M. Tamm*
- 1918.** Stabilization and reactivity of phosphazenes upon oxidation chalcogen elements. **f. garcia**, X. Shi
- 1919.** Dehydrocoupling of phosphines using iron (II) β -diketiminato complexes. A. King, M.F. Mahon, **R.L. Webster**
- 1920.** 1,3,2-Diazaphospholene-catalyzed transfer hydrogenation and hydroboration of unsaturated bonds. **C. Chong**, H. Hiroa*, R. KINJO*
- 1921.** Synthesis and coordination chemistry of a new tetradentate tris(phosphalkene)-phosphine ligand. **P. Miura-Akagi**, C.K. Maile, S.M. Oshiro, M.F. Cain, A.L. Rheingold
- 1922.** Optically active phosphine ligands derived from PH_3 . **C.A. Faradij**, H.A. Sparkes, P.G. Pringle*
- 1923.** Unsymmetrical PNPN-pincer type phosphaphalkene ligands with Rind groups: Synthesis and application to rhodium(II) and iridium(II) complexes. **H. Taguchi**, D. Sasaki, Y. Chang, K. Takeuchi, S. Tsujimoto, T. Matsuo, F. Ozawa*
- 1924.** Streamlined preparation and coordination chemistry of bidentate phosphine-phosphaphalkene ligands. **K.W. Magnuson**, S.M. Oshiro, M.F. Cain, A.L. Rheingold
- 1925.** Photochemistry and reactivity of P_4N_4 cage compounds. **R. Seville Martin**, R.J. Less, D.S. Wright*
- 1926.** P-C bond oxidation via Baeyer-Villiger mechanism. **G. Illic***, D. Vidovic*
- 1927.** Synthesis and coordination chemistry of functionalized phosphine-phosphaphalkene ligands. **S.M. Oshiro**, M.F. Cain
- 1928.** Imidazoles-intercalated α -zirconium phosphate as latent thermal catalysts. **O. Shimomura***, K. Tokizane, T. Nishisako, S. Yamaguchi, J. Ichihara, A. Ohtaka, R. Nomura
- 1929.** From PCl_3 to cationic polyphosphorus compounds. **M. Donath***, J.J. Weigand
- 1930.** Synthesis of chiral crown ethers containing chiral phosphorus atoms. **R. Kato***, Y. Morisaki, Y. Chijo
- 1931.** Phosphonothioate neurotoxin hydrolysis by molybdate complexes. **L.Y. Kuo***
- 1932.** Synthesis and ring-expansion of oxaphosphirane complexes, and their use in O,P,C cage formation. **C. Murcia-Garcia***, R.K. Streubel
- 1933.** Optically active methyl H-phosphinates and its stereospecific transformations to optically active P-stereogenic organophosphoryl compounds. **L. Han***
- 1934.** Synthesis and mechanistic studies towards Gallium substituted pentaphosphides. **F. Hennersdorf***, J.J. Weigand
- 1935.** Chemistry of sodium phosphaethynolate, $\text{Na}[\text{OCP}]$: A rapidly evolving synthon in phosphorus chemistry. **R.J. Gilliard***, J. Protasiewicz, H. Grützmacher
- 1936.** Synthesis of 7,8-dihydro[5]helicenyl phosphines and their application to asymmetric Suzuki-Miyaura coupling. **K. Usui***, K. Yamamoto, T. Shimizu, H. Suemune*
- 1937.** Advancing the chemistry of phosphinines. **J. Wong**, F. Mathey*
- 1938.** Palladacycle catalyzed asymmetric P-H addition of diarylphosphines to *N*-enoyl phthalimides. **R. Chew**, P. Leung*
- 1939.** New catalytic coupling reaction of $>\text{P}(\text{O})\text{H}$ compounds for the preparation of organophosphorus compounds. **L. Han***
- 1940.** Ruthenium catalyzed hydrophosphination of activated alkenes. **R. Belli**, L. Rosenberg*

Hawaii Convention Center
Halls I, II, III

The Expanding Periodic Table: New Discoveries and Chemistry of the Heaviest Elements (#234)

Organized by: Y. Nagame, H. Nitsche, Z. Qin, P. Schwerdtfeger, C. Duellmann, A. Tuerler

Poster Session
19:00 – 21:00

- 1941.** Gas chromatographic behaviors of ZrCl_4 and HfCl_4 in macro- and tracer-scale. **S. Goto***, Y. OSHIMI, K. SHIRAI, K. Ooe, H. Kudo
- 1942.** Liquid-liquid extraction behavior of zirconium and hafnium as homologues of element 104, rutherfordium using chelate extractants. **K. Ooe**, A. Tanaka, R. Yamada, H. Kikunaga, M. Murakami, Y. Komori, H. Haba, S. Goto, H. Kudo
- 1943.** Extraction behavior of Mo and W from H_2SO_4 with Aliquat336 as homologues of seaborgium (Sg). **A. Mitsukai***, A. Toyoshima, M. Asai, K. Tsukada, T.K. Sato, Y. Kaneya, S. Takeda, Y. Nagame, M. Schädel, Y. Komori, M. Murakami, H. Haba, K. Ooe, D. Sato, N. Goto, S. Tsuto

Hawaii Convention Center
Halls I, II, III

Advances in the Medicinal Applications of N-Heterocyclic Carbene Metal Complexes and Azolium Cations (#255)

Organized by: W. Youngs, M. Baker, C. Che, I. Lin, M. Panzner

Poster Session
19:00 – 21:00

- 1944.** Exploring macrocyclic transition metal carbene complexes – toward biosensors for inflammation. **D.J. Woods***, M.K. Taylor
- 1945.** Angiogenic effects of platinum (II) complexes with tridentate N-donor ligands and N-heterocyclic carbene ligands. **S. Fung**, C. Che

Hawaii Convention Center
Halls I, II, III

S-block Metal Chemistry (#304)

Organized by: K. Ruhlandt-Senge, P. Andrews, C. Cui

Poster Session
19:00 – 21:00

- 1946.** Synthesis of an enantiomerically pure methanide and its use as ligand in carbene complexes. **K. Feichtner**, V.H. Gessner*
- 1947.** Investigations of bulky amide ligands for potential incorporation into bimetallic template bases. **M. Fuentes***, R.E. Mulvey, A. Zabala
- 1948.** Ylidies as a link between bis-ylates and methanildes. **T. Scherpf**, R. Wirth, V.H. Gessner*
- 1949.** N-Heterocyclic carbene-stabilised lithium gallates: Synthetic, structural, and reactivity insights. **M. Uzelac**, D.R. Armstrong, A.R. Kennedy, E. Hevia*

* Principle Author

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Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1
The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NO_x Generation, Signaling and Reduction in Biological Systems (#371)

Organized by: N. Lehnert,
G. Richter-Addo, F. Doctorovich,
K. Fujisawa
Presiding: K. Fujisawa

- 19:00 – 1950.** NO binding to H-NOX proteins: Proximal or distal and does it matter? **M. Marletta***
19:30 – 1951. Nitroxyl complexes of non-heme iron centers: Properties and reactivity. **N. Lehnert***, A. Speelman
19:50 – 1952. Hunting nitroxyls and nitroxyls in the elementary steps of biological hydroxylamine oxidation. **K.M. Lancaster***, J.D. Caranto, A. Vilbert
20:10 – 1953. Metalloidothalates and n-heterocyclic carbenes as ligands that support dinitrosyl iron complexes in two redox levels. **M.Y. Daresbourg***, R. Pulukkody, C. Hsieh, P. Ghosh, S. Ding, M. Hall
20:30 – 1954. Nitrogen oxide chemistry with heme-copper and copper complexes: Bioinorganic aspects. **K.D. Karlin**

Hawaii Convention Center
Halls I, II, III

Activation of Small Molecules by Electropositive Metals Related to Chemical Energy Conversion (#380)

Organized by: D. Mindiola,
H. Kawaguchi, L. Schafer, K. Meyer,
A. Veige, M. Reynolds
Presiding: H. Kawaguchi

Poster Session
19:00 – 21:00

- 1955.** Synthesis and reaction study of novel iron dinitrogen complex with iminophosphorane ligand. **T. Suzuki**, H. Masuda, M. Fryzuk, K. Fujimoto, T. Inomata, T. Ozawa
1956. (Iminido)vanadium(V) complex catalysts for olefin insertion/metathesis polymerization. **H. Hayashibara**, K. NOMURA*, X. Hou, A. Ngamnithiporn

Hawaii Convention Center
Halls I, II, III

New Directions for Sensing Metals in Biology (#424)

Organized by: E. New, E. Que,
T. Hirayama

Poster Session
19:00 – 21:00

- 1957.** Highly selective turn-on chemosensor capable of monitoring Zn²⁺ concentrations in living cells and aqueous solution. **K. Bok**, G. You, J. Lee, S. Lee, H. Jang, M. Kim, J. Yun, C. Kim*
1958. Colorimetric sensor for the sequential detection of Cu²⁺ and CN⁻ in fully aqueous media: Practical performance of Cu²⁺. **J. Kim**, S. Lee, Y. Kim, T. Jo, J. Jung, S. Hwang, C. Kim*

- 1959.** Colorimetric chemosensor for the sequential detection of copper ion and amino acids (cysteine and histidine) in aqueous solution. **S. Lee**, G. You, Y. Choi, K. Ryu, S. Hwang, J. Kang, C. Kim*

- 1960.** Development of a new class of high-contrast Fe(II) selective fluorescent probes based on spirocyclic scaffolds and its application. **M. Niwa**, T. Hirayama*, K. Okuda, H.K. Nagasawa*

- 1961.** Red-emitting ratiometric fluorescent probe for Na⁺ based on a benzophosphole P-oxide scaffold. **H. Ogasawara**, M. Tak†, H. Osaki, Y. Sato, K. Ogasawara, T. Higashiyama, S. Yamaguchi*

1962. Water-soluble carboxylic-functionalized chemosensor for detecting Al³⁺ in aqueous media and living cells: Experimental and theoretical studies. **K. Ryu**, Y. Kim, J. Lee, J. Kim, M. Kim, J. Kang, C. Kim*

Sunday Morning

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 3

Experimental and Theoretical Actinide Chemistry: From Fundamental Systems to Practical Applications (#42)

Organized by: J. Gibson,
G. Schreckenbach, T. Yaita, J. Li,
P. Yang
Presiding: G. Schreckenbach, T. Yaita

- 8:00 – 1963.** f-Element complexes of nitrogen-rich ligands: Precursors to highly porous f-element nitride and oxide foams for nuclear fuel applications.

J.M. Heathauer*, J.L. Kipling, B.C. Tappan, N.J. Henson, N. Travia, K. Brown, K. Maerke

- 8:20 – 1964.** Exploring photochemistry of uranyl(VI). **S. Tsushima***

8:50 – 1965. Study of complexation of Pu(IV) and Th(IV) with glutarimidedioxime by potentiometry, spectrophotometry and X-ray analysis. **G. Tian***, S. Yang, L. Xiang, S. Teat, D.K. Shuh

- 9:20 – 1966.** Insights in actinide chemistry through integration of computational modeling and experiments.
W.A. de Jong, J. Gibson, Y. Gong, M. Van Stipdonk, S. Odoh

9:50 Break

- 10:05 – 1967.** Exploring the structure and behavior of uranyl species in the gas phase using tandem mass spectrometry. **M. Van Stipdonk**, A. Plaviak, C. O'Malley, J. Gibson

- 10:35 – 1968.** Recent investigations of solid state chemistry of lanthanides and actinides in Soochow University. **S. Wang***

- 11:05 – 1969.** Fundamental studies of actinides on solid-phase mesoporous materials. **E.C. Uribe***, T. Parsons-Moss, J. Shusterman, H. Mason, H. Nitsche

- 11:25 – 1970.** Study of extraction behavior mechanism of uranyl peroxy cage clusters in mesoporous silica SBA-15.
Y. Liu*, A. Czarnecki, J. Szymanowski, G. Sigmon, P.C. Burns

Hilton Hawaiian Village
Mid-Pacific Center, Coral 1

Metal-Organic Frameworks: Synthesis, Properties and Applications (#50)

Organized by: G. Shimizu, J. Long,
M. Suh, Q. Xu, X. Chen

- 8:00 – 1971.** Design strategies for the construction of functional metal-organic frameworks. **M. Eddaoudi**

- 8:20 – 1972.** New synthetic approaches for MOF preparation. **H. Zhou***

- 8:50 – 1973.** Top-down generation and screening of metal-organic frameworks for gas storage and separation applications. D.A. Gomez-Gualdrón, Y.J. Colón, Y.G. Chung, **R.Q. Smur***

- 9:10 – 1974.** AuToGraFS: Automatic topological generator for framework structures. M.A. Addicoat*, D.E. Coupy, **T. Heine**

- 9:25 – 1975.** Metal-organic frameworks impregnated with nanoparticles of metals and metal compounds. **M. Suh***, D. Lim, K. Cho

- 9:45 – 1976.** Leach-free catalysis and electroactive materials from metal-thiolate-enabled porous frameworks. **Z. Xu***, K. Yee, M. Zeller

- 10:00 – 1977.** Linker exchange reaction mechanisms in MOFs and its application toward the synthesis of hybrid catalyst systems. **J.A. Byers***, C. Tsung, Z. Li, J. Morabito, L. Chou

- 10:15 – 1978.** Computer modeling of proton conduction in metal-organic frameworks. **F. Paesani**

10:35 – 1979. Development of visible-light-responsive photocatalysts based on designability of PCP/MOFs. **Y. Horuchi***, K. Miyahara, T. Toyao, M. Matsuoka

- 10:50 – 1980.** Porous materials for energy and environmental applications. **P. Thallapally**

11:10 – 1981. Water stable MOFs for carbon capture. **G. Shimizu**, J. Lin, R. Vaishyanathan, F. Akhtar, T. Woo, R. Mah, H. Dureckova

11:30 Closing remarks

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

From Pnictides to Perovskites: Impact of Local Structure in Solid State Chemistry (#62)

Organized by: H. Kageyama,
B. Kennedy, J. Wiley
Presiding: M. Bieringer, B.J. Kennedy,
T. Mori, K.R. Poeppelmeier

- 8:00 – 1982.** Impact of chemical pressure on room-temperature ferromagnetism in cubic perovskite Sr_{1-x}Ba_xCoO₃. **H. Sakai***

- 8:20 – 1983.** High pressure synthesis, structure, and magnetic properties of novel perovskite oxyhydrides. **C. Tassel***, Y. Goto, Y. Kuno, Y. Kobayashi, H. Kageyama

- 8:40 – 1984.** Oxygen storage capacities of BaRuO₃ polytypes. **Y. Shirako***, K. Kobayashi, K. Niwa, H. Kojitani, M. Akaogi, M. Ozawa, M. Hasegawa

- 9:00 – 1985.** Structural and electrical properties of ferroelectric complex perovskite solid solutions based on Bi(Zn_{2/3}Nb_{1/3}O₃)₃. **A. Paterson**, H. Wong, Z. Ye

- 9:20 – 1986.** Systematic charge distribution change in BiMo₃ and PbMo₃ (M: 3d transition metal). **M. Azuma***

9:55 Break

- 10:00 – 1987.** Synthesis and structural study of Pb containing oxyfluoride. **K. Oka**, K. Ohishi

- 10:20 – 1988.** Local structures in typical perovskite materials. **Y. Liu**

- 10:55 – 1989.** Thermally-induced layer compression in the topochemically-prepared Fe₆₂Ti₁₀O₁₀. L. Lustin, Y. Hosaka, T. Aharen, C. Tassel, Y. Shimakawa, H. Kageyama, **J.B. Wiley***

- 11:15 – 1990.** Ordered oxifluorides with anti-perovskite structures Thomas Vogt University of South Carolina. **T. Vogt***

- 11:35 – 1991.** Dimensionality of thermoelectric transport and electronic structures in layered complex nitrides. **I. Ohkubo***, T. Mori

11:55 Closing remarks

Hilton Hawaiian Village
Rainbow Tower, Rainbow 2

Accessing the Full Potential of Redox-Active Ligands: Reactivity and Applications (#87)

Organized by: T. Storr, C. Grapperhaus, H. Fujii
Presiding: C.A. Grapperhaus

- 8:00 – 1992.** Synthesis, characterization, and reactivity of redox-active aluminum-nitroxide complexes. A.M. Poitras, T. Herb, J.A. Bogart, P.J. Carroll, E.J. Schelter, C.R. Graves*

- 8:20 – 1993.** Redox-active ligand induced single-electron reactivity on closed-shell noble metals. **J. van der Vlugt***

- 8:40 – 1994.** Ligand-based redox chemistry in complexes of oligopyrrolid fragments. **E. Tomat***, R. Gautam

- 9:00 – 1995.** The taco and the pancake: Structural and spectroscopic signatures of ligand noninnocence in metallocorroles. **A. Ghosh**

- 9:30 – 1996.** Redox chemistry of palladium complexes containing redox-active ligands: Driving on the wrong side of the road? **R. Hicks**, C.A. Sanz

- 10:00 – 1997.** Oxidized metal phenoxide complexes - correlation of electronic structure and reactivity. **T. Storr***, R. Clarke, L. Chiang

10:30 Break

- 10:40 – 1998.** Functional materials based upon ferrocene. J. Qu, W. Ji, H. Zhou, S. Jing*

- 11:00 – 1999.** Effect of Lewis acids on oxidation states of transition-metals.

M. Swart*, A. Castro, A. Romero-Rivera

- 11:20 – 2000.** Radical gold dithiolen complexes: Structural and electronic consequences of a fully non-innocent ligand. K. Mebruk, F. Camerer, T. Higashino, T. Mori, **M. Fourmigue***

- 11:40 – 2001.** High-valent manganese and cobalt complexes with redox-active salen ligands related to asymmetric catalysis. **T. Kurahashi***, H. Fujii*

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Chemistry and Application of Boron Clusters (#152)

Organized by: S. Kang, N. Hosmane, D. Schubert, H. Nakamura, Z. Xie
Presiding: Z. Xie

- 8:00 – 2002.** Discovery of carboranylphenoxycacetanilides as inhibitors of heat shock protein (HSP) 60 chaperone activity. **H. Nakamura***

- 8:30 – 2003.** Aromatic-ring-fused benzocarboranes and their *nido*-species. **K. Nishino**, Y. Chujo*, Y. Morisaki

- 8:50 – 2004.** Design and synthesis of m-carborane and MAGMAS inhibitor conjugated novel hybrid compounds as potential therapeutics for the treatment of renal cell carcinoma. **S. Das**, N.S. Hosmane, B.C. Das*, P.V. Veldhuizen

9:20 Break

- 9:30 – 2005.** Carboranes in medicinal chemistry. **E. Hey-Hawkins***, W. Neumann, R. Kuhnert, R. Frank, B. Schwarze, S. Boehnke, V. Ahrens, A. Beck-Sickinger

- 10:00 – 2006.** Highly efficient synthesis of small-diameter boron nitride nanotubes from h-BN. **B. Simard***, K. Kim, C. Kingston, M.J. Jakubinek, J. Guan, R. Iannitto, S. Walker, M. Plunkett

- 10:20 – 2007.** Transition metal-promoted cyanation and carboxylation of C₂B₁₀-CB₁₁, and CB₉ carboranes. **M. Juhasz***

10:40 Break

- 10:50 – 2008.** Finding of deboronation reaction of *ortho*-carborane derivatives catalyzed by metal ions and its application to ¹³B NMR probes. **t. tanaka***, Y. Nishihara, R. Araki, T. Saido, R. Abe, S. Aoki

- 11:10 – 2009.** Nanostructured boron compounds: Applications in cancer therapy. **N.S. Hosmane***

11:40 Closing Remarks

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Current Trends and Interconnectivities Among Fundamental and Applied Inorganic Fluorine Chemistry (#156)

Organized by: K. Matsumoto, R. Hagiwara, G. Schrobilgen, H. Mercier, R. Syvert
Presiding: K. Matsumoto

- 8:00 – 2010.** Topochemical reactions of perovskite-based transition-metal oxyfluorides. **H. Kageyama***

* Principle Author

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Final Pacificifchem 2015 program online at:

<http://pacificifchem.org/onlineprogram>

- 8:30 – 2011.** Exploring the $\text{Sm}_{1-x}\text{Ca}_x\text{F}_{3-x}$ and $\text{La}_{1-x}\text{Ba}_x\text{F}_{3-x}$ solid solutions as solid state electrolytes: Relationships between structural features and F-ionic conductivity. **A. Demourgues***, B. Dieudonne, J. Chable, E. Durand, F. Mauvy, S. Fourcade, V. Maisonneuve, C. Legein, M. Body
- 9:00 – 2012.** Enhanced dispersion stability and photocatalytic activity of TiO_2 particles fluorinating by fluorine gas. **J. Kim***, S. Yonezawa, H. Kinoshita, M. Takashima
- 9:20 – 2013.** Ionic liquid fluorosulfonylamides as electrolytes for rechargeable sodium ion batteries. **R. Hagiwara***, T. Nohira, K. Matsumoto, C. Ding, C. Chen, A. Fukunaga*, Sakai, K. Nitto
- 9:40 Break**
- 9:55 – 2014.** Simple fluorinated precursors and methods for electrolyte components of lithium-ion batteries. **G. Roessenthaler***, N. Kalinovich, M. Winter
- 10:25 – 2015.** Fluorinated carbon nanoparticles for primary Li battery. **G. Henri***, a. tressaud, e. durand, S. Leclerc, A. PORRAS GUTIERREZ, K. Le Van
- 10:55 – 2016.** $\text{K}[\text{BF}(\text{CN})_3]$ – synthesis and chemistry of a mixed cyanofluoroborate. **M. Finze***, J. Landmann, J. Sprenger, N. Ignat'ev, E. Bernhardt, H. Willner
- 11:25 – 2017.** Anion exchanging and interlayer distance control of layered double hydroxide synthesized by liquid phase deposition. **M. Mizuhata***, M. Inoue*, H. Maki*
- 11:45 Closing Remarks**

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 2

Advances in Phosphorus Chemistry: Materials, Reactivity at Phosphorus, and Synthesis (#226)

- Organized by:* R. Waterman, F. Ozawa, D. Gates, P. Leung
Presiding: R. Waterman
- 8:00 – 2018.** New advances in the chemistry of monovalent phosphorus. **F. Mathey***
- 8:20 – 2019.** Electrophilic phosphonium cations in Lewis acid catalysis. **D. Stephan***
- 8:40 – 2020.** Earthly chemistry of interstellar phosphorus-containing molecules. A. Velian, M. Nava, W. Transue, C. Cummins, C. Womack, J. Jiang, R. Field
- 9:00 – 2021.** P-Chemistry – from activating P_4 to catalysis. **K. Lammertsma***
- 9:20 – 2022.** Zwitterionic diphosphanides. **J.J. Weigand***
- 9:40 – 2023.** Geometric deformation as a design principle in organophosphorus catalysis. **A.T. Radosevich**
- 10:00 – 2024.** "Inorganic" arylphosphines. J.A. Bailey, H.A. Sparkes, C.A. Faradj, P.G. Pringle*
- 10:20 – 2025.** Understanding and expanding the synthesis of sterically-hindered trialkylphosphines. **D. Amoroso***, J. Dyck, M. Humeniuk, A. Melaragni, M. Moser, S. Zavorine
- 10:40 – 2026.** All things P: New investigations into multidentate, non-innocent, and/or chiral phosphines and phosphaphalkene-based ligands. **M.F. Cain***
- 11:00 – 2027.** Interactions of phosphazene superbases with simple Lewis acids and their frustrated Lewis pair capabilities. N.A. Johnson, B.S. Thome, P.O. Wagers, B.D. Wright, M.J. Panzner, W. Youngs, C.A. Tessier*
- 11:20 – 2028.** Activation and functionalization of elemental phosphorus. **M. Peruzzini***
- 11:40 – 2029.** Carbone-phosphorus chemistry: The recent developments. **D. Vidovic**

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

The Expanding Periodic Table: New Discoveries and Chemistry of the Heaviest Elements (#234)

- Organized by:* Y. Nagame, H. Nitsche, Z. Qin, P. Schwerdtfeger, C. Duellmann, A. Tuerler
Presiding: P. Schwerdtfeger, A. Türler
- 8:00 – 2030.** Atomic properties of super-heavy elements. **V. Dzuba***
- 8:30 – 2031.** Studies of the heaviest elements with SHIPTRAP. **M. Block***
- 9:00 – 2032.** First ionization energies of heaviest actinides, lawrencium and nobelium. **T.K. Sato***
- 9:30 – 2033.** Relativistic coupled cluster calculations of atomic properties of the heaviest elements. **A. Borschevsky***, U. Kaldor, E. Elav
- 10:00 – 2034.** Electrochemistry of the heaviest elements at JAEA. **A. Toyoshima***
- 10:30 – 2035.** Heavy element research at Texas A&M University. **C.M. Folden***
- 11:00 – 2036.** Extraction behavior of a cat-ionic fluoride complex of rutherfordium with a TTA chelate extractant from HF/HNO_3 acidic solutions. **A. Yokoyama***, Y. Kitayama, Y. Fukuda, H. Kikunaga, M. Murakami, Y. KOMORI, H. Haba, K. Tsukada, A. Toyoshima

- 11:30 – 2037.** Solid-liquid and liquid-liquid extractions of Zr, Hf, Th and element 104, Rf, in an Aliquat 336/HCl system. **Y. Kasamatsu***, T. Yokokita,

- Y. Shigekawa, A. Kino, K. Nakamura, Y. Yasuda, K. Toyomura, N. Takahashi, H. Haba, Y. Komori, M. Murakami, Y. Kuboki, T. Yoshimura, A. Shinohara

S-block Metal Chemistry (#304)

- Organized by:* K. Ruhlandt-Senge, P. Andrews, C. Cui
Presiding: K. Henderson

- 8:00 – 2038.** Supersized triple-decker organometallic sandwiches formed by highly charged π -bowls with mixed alkali metal cores. **M.A. Petrukhina***

- 8:30 – 2039.** Double deprotonation at a single carbon center: Methanides and ylidides as unique carbon ligands. **V.H. Gessner***

- 9:00 – 2040.** Impact of metal choice in forming mono- and bimetallic chiral alkali metal amides: Anion rearrangements and ligand modification processes. **P. Andrews**

9:30 Break

- 9:40 – 2041.** Pre-organized base approaches to arene and related metallation chemistry. **R.E. Mulvey***, C. O'Hara, A.J. Martinez-Martinez

- 10:10 – 2042.** Alkali metal hydride complexes: Well-defined molecular species of saline hydrides. **A. Stasch***

- 10:40 – 2043.** Developing group 1 dihydro-pyridine chemistry: From transient intermediates to isolable compounds. **S. Orr***, R.E. Mulvey, S.D. Robertson, J.J. Liggett, R. McLellan, A.R. Kennedy

- 11:10 – 2044.** Recent developments in lanthanoid pseudo-Grignard reagent chemistry. **P.C. Junk***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NO_x Generation, Signaling and Reduction in Biological Systems (#371)

- Organized by:* N. Lehnert, G. Richter-Addo, F. Doctorovich, K. Fujisawa
Presiding: F. Doctorovich

- 8:00 – 2045.** Kinetics studies of the formation and reactions of dinitrosyl iron complexes with cysteine in aqueous solution. **P.C. Ford***, J. Pereira, R. Han
- 8:30 – 2046.** Behavior of redox-active NO ligands on dinuclear ruthenium complexes. **Y. Arikawa***

- 9:00 – 2047.** Elucidating the conformational dynamics and regulatory interactions in nitric oxide synthases. **C. Feng***, Y. Sheng, A. Astashkin

- 9:20 – 2048.** Mechanistic studies of nitric oxide reduction by denitrifying NO reductases and heme-nonheme diiron containing myoglobin constructs. **P. Moënne-Locoz***, H. Matsumura, Y. Lu, S. de Vries

- 9:50 Break**
- 10:00 – 2049.** Nickel nitrosyl complexes supported by a PEP ligand. **J. Gwak**, Y. Kim, Y. Lee*

- 10:20 – 2050.** Cryptic noninnocence: FeNO triarylcorroles are not $\{\text{FeNO}\}_6^6-$. H. Vasquez-Lima, H. Norheim, **A. Ghosh***

- 10:40 – 2051.** Iron and cobalt nitrosyl involved in NO_x transformations. **T. Harrop***

- 11:00 – 2052.** Inner-sphere proton-coupled electron transfer as a key mechanism for nitroxyl (HNO) generation modulated by metal centers or hydrogen sulfide (H_2S). **I. Ivanovic-Burmazovic**

- 11:30 – 2053.** Interactions of N_xO_y species with synthetic metalloporphyrins and heme proteins. **G.B. Richter-Addo***

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Activation of Small Molecules by Electropositive Metals Related to Chemical Energy Conversion (#380)

- Organized by:* D. Mindiola, H. Kawaguchi, L. Schafer, K. Meyer, A. Veige, M. Reynolds
Presiding: H. Kawaguchi, M.A. Reynolds

8:00 opening remarks

- 8:05 – 2054.** Small molecule activation mediated by an iron half-sandwich complex, $[\text{Cp}^*\text{Fe}]_2$. **M.D. Walter**, M. Reiners, M. Maekawa, M. Freytag, P. Jones, J. Hohenberger, J. Sutter, K. Meyer

- 8:25 – 2055.** Rationally designed pincer platforms for rare earth metals. **P.G. Hayes***

- 8:45 – 2056.** Reductive activation of CO_2 and related small molecules across a Ti-Ti double bond. **G. Cloke***

- 9:05 – 2057.** C-H functionalization of simple hydrocarbons mediated by tungsten allyl nitrosyl complexes. **R.A. Baillie**, P. Legzdins*

- 9:25 – 2058.** Highly active MnN-Li₂NH composite catalyst for ammonia decomposition. **J. Guo**

9:45 break

- 10:00 – 2059.** Reactivity of titanium-hydrido complexes from a computational perspective. **E. Clot***

- 10:20 – 2060.** Activation and functionalization of metal-metal multiple bonds. **Y. Tsai***

- 10:40 – 2061.** Activation of small molecules by chelating triamido uranium complexes. **S.T. Liddle**, B. Gardner, D. King, P. Cleaves, D. Patel, J. McMaster, E. McInnes, N. Chilton, F. Tuna, W. Lewis, A. Blake, L. Maron, C. Kefalidis

- 11:00 – 2062.** Small molecule activation by complexes of low-valent f elements. **M. Mazzanti***

- 11:20 – 2063.** Activation of dinitrogen by a vanadium complex bearing a chelating bis(phenoxide)-aniline ligand. **H. Kawaguchi***

11:40 concluding remarks

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 3

New Directions for Sensing Metals in Biology (#424)

- Organized by:* E. New, E. Que,
T. Hirayama
Presiding: E. New

- 8:00 – 2064.** Development of far-red to near-Infrared small-molecule fluorescence probes for monitoring dynamics of calcium ion. **K. Hanaoka***
- 8:30 – 2065.** Design of dual emission fluorescent probes for metal ions based on arene-metal ion contact and their application to cell bioimaging. **A. Ojida***

- 9:00 – 2066.** Design of a red-emitting ratio-metric fluorescent probe for the detection of intracellular sodium ion. **M. Taki***

- 9:20 – 2067.** Development of ratio-metric strategies for sensing labile metal pools in biology. **C. Shen***, J. Kolanowski, E. New, A. White

9:40 Morning tea

- 10:20 – 2068.** Inorganic chemistry in control of cell fate decisions: Probes for understanding how zinc fluxes regulate mammalian fertilization. **T.V. O'Halloran**

- 10:50 – 2069.** In situ fluorescence imaging of biological trace metals. **C. Fahrni***

- 11:20 – 2070.** New optical indicators for neuronal activity. **E. Miller**

- 11:40 – 2071.** Development and applications of fluorescent probes for selective and turn-on detection of $\text{Fe}(\text{II})$ ion.

- T. Hirayama***, M. Niwa, K. Okuda, H.K. Nagasawa

MACR

Area 3 – Macromolecular

Tuesday Morning

Hawaii Convention Center
325B

Synthetic Biopolymers (#37)

- Organized by:* T. Deming, Z. Li, T. Kaneko
Presiding: T. Deming, T. Kaneko, Z. Li

8:00 Introductory Remarks

- 8:05 – 1.** Endowing protein biopolymers with intelligence. **J.K. Montclare**, **J.A. Frezzo**

- 8:40 – 2.** Assisted protein refolding by artificial molecular chaperones. **L. Shi***

- 9:15 – 3.** Photoswitchable rapid prototyping of heterotypic cell-cell contacts and cell motility assay. R. Andrews, K. Mun, G. Kumar, **C. Ho**, C. Co

- 9:35 – 4.** Biocjugates of fluorinated azobenzene. **W. Brittain***

9:55 break

- 10:10 – 5.** Poly(oligonucleotide): Development and biomedical applications for nucleic acid-programmed polymers and nanoparticles. **N. Gianneschi**

- 10:45 – 6.** Polyphosphoester: From controlled synthesis to biomedical applications. **J. Wang***

- 11:20 – 7.** Facile synthesis and applications of site-specific protein-polymer conjugates. **H. Lu***

- 11:40 – 8.** Synthesis and blood compatibility of sequence-specific polymers via regioselective ROMP. **S. Kobayashi**, k. fukuda, K. Herai, M. Kataoka, K. Osawa, M. Tanaka*

* Principle Author

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Hawaii Convention Center
323B

Polymer Gels as Advanced Soft Materials (#83)

Organized by: R. Yoshida, T. Miyata, F. Winnik, J. Aizenberg
Presiding: F. Winnik, R. Yoshida

8:00 Opening Remarks

8:05 – 9. Slide-ring materials: novel concept for flexible tough polymers. **K. Ito***

8:35 – 10. Photo-polymerized networks based on the copper-catalyzed azide-alkyne (CuAAC) reaction. **C.N. Bowman***, A. Baranek, H. Song, A. Alzahrani, M. McBride, T. Gong

9:05 – 11. Controlled cross-linking strategy for formation of hydrogels, microgels, and nanogels. J. Zhang, X. Wang, L. Wang, F. Yang, **D. Wu***

9:25 – 12. Onion-like polymer capsules with multiple concentric shells. **B.C. Zarket***, S. Antczewski, T. Coyne, J. Heckelman, **S.R. Raghavan***

9:45 Break

10:00 – 13. Structure and properties of defect-controlled polymer gel. **M. Shibayama***, K. Nishi, T. Sakai

10:30 – 14. Reprocessable silicone boronate gels. **M.A. Brook**, L. Zepeda-Velasquez, C. DeWolf, E. Mansuri, M.E. Whinton

11:00 – 15. Wide bicontinuous compositional windows from co-networks made with telechelic macromonomers. **G. Tew**

11:20 – 16. Understanding the fibrillation of self-assembled low molecular weight hydrogelators. **D. Hermida-Merino***, G. Portale

11:40 – 17. Theoretical and computational modeling of structure and dynamics of oligomeric electrolyte based multisolvent gelators. **A.E. Kobryn**, S. Gusalov, A. Kovalenko

Hawaii Convention Center
326B

Simulation of Polymers (#110)

Organized by: Y. Masubuchi, S. Shanbhag, V. Vao-soongnern, C. Baig
Presiding: S. Shanbhag, S. Sukumaran

8:00 – 18. Density functional theory for excluded volume effects in polymer brushes. **C. Chen**, P. Tang, F. Qiu*, A. Shi

8:20 – 19. Density functional tight binding study of defected α and γ nylon6. S. Arabnejad*, **S. Manzhos**

8:40 – 20. Fast lattice Monte Carlo simulations of polymers. **Q. Wang***

9:00 – 21. Toward robust self-diffusivity estimates in complex fluids. **S. Shanbhag***

9:20 – 22. Rotational motion of polymer chains under simple shear flow. **J. Takimoto***, S. Sukumaran, K. Mori, A. Fukuhara

9:40 – 23. Stretch/orientation induced reduction of friction of polymers. **Y. Masubuchi***

10:00 – 24. Primitive path analysis of entanglements in polymer blends. **S. Sukumaran***, J. Takimoto

10:20 – 25. Multi-million-atom molecular dynamics simulations of conformational dynamics in polymer nanoparticle composites using explicit solvent treatment. **S. Sankaranarayanan**, S. Deshmukh

10:40 – 26. Large scale coarse-grained molecular simulations on fracture process of rubber. **M. Oikawa**, R. Sakamaki, Y. Bito, S. Ueno, M. Naito, H. Kishimoto, Y. Masubuchi*

11:00 – 27. Multiscale simulation for polymer nanocomposites. **T. Ozawa***, K. Ohata, M. Watanabe, G. Goldbeck, V. Regnier

11:20 – 28. Improving composite materials via molecular simulations of epoxy cross-linking at carbon fibre interfaces. B. Demir, **T.R. Walsh***

11:40 – 29. Coarse-grained simulation study of the filler filled materials using OCTA system. **H. Morita**, K. Hagita

Hawaii Convention Center
324

Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112)

Organized by: M. Kamigaito, C. Hawker, G. Qiao, K. Wooley, E. Yashima
Presiding: C. Boyer, C.J. Hawker

8:00 – 30. Precision functional polymers by precision radical polymerization. **M. Sawamoto***

8:30 – 31. Application of photoinduced electron transfer (PET) for the synthesis and post-modifications of well-defined polymers. **C. Boyer***, J. Xu, S. Shamugam

9:00 – 32. Precision synthesis of stimuli-responsive polymers via living/controlled cationic polymerization. **S. Aoshima***, S. Kanaoka, A. Kanazawa

9:30 – 33. Reversible mechanistic transformation of growing nature during vinyl polymerizations. **K. Satoh***, M. Kamigaito

10:00 – 34. Bioinspired supramolecular architectures. **S. Stupp***

10:30 – 35. Intramolecular catalyst transfer behavior depending on transition metal catalysts in the synthesis of conjugated polymers and copolymers. M. Nojima, Y. Ohta, T. Yokoza*

11:00 – 36. Methods to synthesize well-defined polyesters with control of sequence, regio- and stereochemistry. **A.M. DiCiccio**, J. Longo, G. Coates

11:15 – 37. Synthesis and fundamental properties of poly(*ortho*-phenylene)s. **K. Mikami***, Y. Mizukoshi, Y. Okada, M. Uchiyama*

11:30 – 38. Controlling polymer conformations: Efficient synthesis of shape-persistent ladder polymers via annulation ladder polymerization. **Y. Xia***

11:45 – 39. Rational strategy for the realization of chain-growth supramolecular polymerization. **D. Miyajima***, K. Jiheong, T. Aida*

Hawaii Convention Center
323C

Characterization of Polymers and Polymer Assemblies in Solution (#172)

Organized by: T. Sato, T. Yoshizaki, T. Chang, J. Mays, C. Wu
Presiding: T. Chang, J. Mays, T. Sato, T. Yoshizaki

8:00 Introductory Remarks

8:05 – 40. Local conformation and intermolecular interactions of rigid cyclic amylose carbamate derivatives. **K. Terao**

8:50 – 41. Residual contribution of three-segment interactions to the second virial coefficient for unperturbed ring polymers. **D. Ida***, T. Yoshizaki

9:35 – 42. Effects of shape on the solution properties of polymers. A computational approach. **B.A. Pazmino Betancourt**, J.F. Douglas

10:05 – 43. Long-chain branching analysis of comb-shaped polystyrenes. **S. Lee***, T. Chang

10:35 Break

10:50 – 44. Picture of dilute solution behavior of polymers through polyelectrolyte simulation. **T. Yoshizaki**, H. Yamakawa, D. Ida

11:20 – 45. Theoretical study of network formation and mechanical property of physical gel with well-defined junction structure. **H. Ozaki***, T. Koga

Hawaii Convention Center
325A

Functional Materials Based on Organic-inorganic Hybrid Polymers (#221)

Organized by: K. Naka, F. Jaekle, C. Ha, J. Ohshita
Presiding: C. Ha, F. Jaekle, K. Naka, J. Ohshita, Y. QIN

8:00 Opening Remarks

8:05 – 46. New hybrid materials based on element-blocks. **Y. Chujo***

8:35 – 47. Platinum-containing conjugated polymers with novel structures and properties. **Y. QIN***

8:55 – 48. Metallo-supramolecular polymers as stimuli-responsive materials. **S.J. Rowan***

9:15 – 49. Multifunctional supramolecular nanotubes and nanoparticles as sensory and delivery vehicle. **C. Kim***, J. Lee

9:35 – 50. Stimuli-responsive metallosupramolecular polymers. **C. Weder***

9:55 Break

10:05 – 51. Synthesis and application of polysilsesquioxanes as element-blocks. **T. Gunji**

10:25 – 52. Pyridylborates as a new ligand platform for metal-containing polymers and metallo-supramolecular materials. **F. Jaekle***

10:45 – 53. Supramolecular polymerization of fullerene via molecular recognition. **T. Haino***

11:00 – 54. Organic-inorganic hybrid polymers based on nickel(II) complexes of Goedken's macrocycle. **J.A. Paquette**, E.R. Sauve, J.B. Gilroy*

11:15 – 55. Development of polysilsesquioxane aerogels and xerogels with improved mechanical properties. **K. Kanamori**, T. Shirizu, K. Nakaniishi

11:30 – 56. Synthesis of network polymers using cubic silsesquioxane and their discriminating properties for the particle size. **T. Kakuta***, K. Tanaka, Y. Chujo

11:45 – 57. Modification of PET and PEN film surfaces by organic-inorganic hybrid polymer thin films. **T. Tamai***, M. Watanabe, Y. Kobayashi, K. Mitamura, K. Matsukawa

Hawaii Convention Center
327

Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281)

Organized by: M. Cunningham, M. Sawamoto, P. Chamagne, J. Rawlins
Presiding: P. Champagne

8:00 Opening Remarks

8:05 – 58. Next generation aliphatic polyester block polymers: Design, synthesis, and performance. **M. Hillmyer**

8:35 – 59. Copolymers of lactide with aliphatic cyclic esters: From thermoplastic elastomers to functional poly(lactic acid)s. **M. Shaver***

9:05 – 60. Capturing CO₂ for cellulose dissolution and derivation. **H. Xie**, Y. Yang, L. Song, X. Yuan, C. Yuan, Q. Zhen

9:25 – 61. Aerogels from biopolymers and biomonomers. **D.A. Schiraldi**

9:45 – 62. Development of stereo-block polyactides: An approach to high-performance polyactide materials. **Y. Kimura***, K. Masutani

10:15 – 63. Carbon dioxide switchable cellulose nanocrystals. H. Wang, J. Bouchard, P. Champagne, P.G. Jessop, M. Cunningham*

10:35 – 64. Organocatalytic polymerization of biodeered bifunctional acyclic and heterocyclic monomers. **E. Chen**

11:05 – 65. Efficient, chemical-catalytic approach to the production of renewable monomers succinic acid and 3-hydroxypropanoic acid from biomass. **M. Mascali***, L. Wu, s. dutta

11:25 – 66. Functional biobased elastomers from *Eucommia ulmoides*. **U. Hiroshi**

Hawaii Convention Center
323A

Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319)

Organized by: X. Zhang, Q. Guo, W. Qin, T. Hu, K. Ramasamy
Presiding: X. Zhang

8:00 Discussion by Keith Moo Young

8:25 – 67. Enabling bio-based economy: Hybrid approaches for lignin valorization. **S. Singh**

8:45 – 68. Biopolymeric ionic liquids (bio-PILs): A materials family originated from lignin and its applications in CO₂ capture. **C. Vriamont***, J.P. Hallett, G.J. Britovsek

9:05 – 69. Role of lignin in a biorefinery. **T. Yuan***, S. Yang*, R. Sun*

9:25 – 70. Developing biobased adhesives by chemical coupling lignin to biopolymers. **N. Hatii***, W. Grigsby, J. Jin, N. Edmonds

9:45 BREAK

9:55 – 71. Deep eutectic solvents (DES) for lignin extraction. **X. Zhang***

10:15 – 72. Lignin-derived nanoporous carbon spheres@CuFeS₂ composite: Synthesis and thermoelectric properties. **D. Liang***

10:35 – 73. Commodity-scale phytochemicals from the lignocellulose of mega-crops. **S.A. Miller***

10:55 – 74. Mechanistic look at lignin sulfonation. **R. Beatson***

11:15 – 75. Catalytic solvolysis features of lignin fractions with different molecular weight distribution. **J. Kim***, S. Park, S. Oh, J. Park, D. Shin, J. Choi

11:35 – 76. Catalytic conversion of biomass to fuels and value-added chemicals via platform molecules. **Q. GUO***

Hawaii Convention Center
326A

Polymers for Energy and Optoelectronic Devices (#361)

Organized by: K. Oyaizu, R. Advincula, D. Choi
Presiding: D.H. Choi, K. Oyaizu

8:00 Introductory Remarks

8:05 – 77. High-performing organic semiconducting polymers for electronics and optoelectronics. **D.H. Choi***, M. Cho, J. Shin, D. Lee, H. Um

8:25 – 78. High performance organic thin film transistors based on conjugated polymers containing benzobisthiadiazole and its related heterocycles. **Y. Wang**, T. Michinobu

8:40 – 79. Novel thienoacene-based semiconducting materials for organic solar cells and field effect transistors. **M. Wong***, Z. Li, K. Zhang, B. Wang

8:55 – 80. Development of 4,7-dialkylated phenanthrodi thiophene-based semiconducting polymers and their application to high-performance solar cells. **H. Mori**, R. Takahashi, K. Hyodo, H. Nonobe, Y. Nishihara*

9:10 – 81. Synthesis and characterization of pyrenobisthiadiazole-based semiconducting polymers. **W. Kaneshika***, H. Nonobe, R. Takahashi, H. Mori, Y. Nishihara*

9:25 – 82. Optimization of side chains in phenanthrodi thiophene-isodindigo copolymers: Relationships between thin-film structure and device performance. **S. Nishinaga**, H. Mori, Y. Nishihara*

9:40 Break

9:50 – 83. Semi-crystalline photovoltaic polymers with noncovalent Coulomb interactions for highly efficient polymer solar cells. **H. Woo***

*** Principle Author**

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- 10:20 – 84.** Conjugated polymers for highly efficient solar cells: Fundamental understanding on PBDT-FTAZ. **W. You***
- 10:35 – 85.** High-performance semiconducting polymers incorporating naphtho-bis(chalcogenodiazoles for polymer solar cells. **I. Osaka**, K. Kawashima, K. Takimiya
- 10:50 – 86.** Efficiency-limiting processes in low-bandgap donor: perylene diimide photovoltaic blends. **D.W. Gehrig**, A. Sharenko, A. Kyaw, S. Roland, D. Neher, T. Nguyen, F. Laqua*
- 11:05 – 87.** Characterization of molecular aggregation structure in polymers with perylene diimide side-chain. **M. Kido**, S. Nojima, R. Ishige, Y. Kim, B. Ree, Y. Ko, N. Ohta, K. Kojo, M. Ree, T. Hirai, A. Takahara
- 11:20 – 88.** Side chain engineering of naphthalenediimide-bithiophene (NDI-T2)-based N-type polymers for efficient all-polymer solar cells. **W. Lee***, C. Lee, B. Kim

Tuesday Afternoon

Hawaii Convention Center
325B

Synthetic Biopolymers (#37)

- Organized by:* T. Deming, Z. Li,
T. Kaneko
Presiding: T. Deming, T. Kaneko, Z. Li
- 13:00** Introductory Remarks
- 13:05 – 89.** Biobased functional polymers from plant oils. **U. Hiroshi**
- 13:40 – 90.** Preparation of biobased polyimides from 4-aminocinnamate and their optoelectronic properties. **J. singh***, P. SUVANNASARA, S. TATEYAMA, T. Kaneko
- 14:00 – 91.** Bio-inspired adhesive polymers for energy storage devices. **H. Lee***
- 14:35** Break
- 14:50 – 92.** Anti-inflammatory and antibacterial coatings derived from biological polyphenols. T. Sileika, D. Barrett, **P. Messersmith***
- 15:25 – 93.** Synthesis of polyalactides bearing antibacterial moiety at chain end. **H. Ajiro**, S. Ito, M. Akashi*
- 15:45 – 94.** Super-engineering plastics from exotic amino acids. **T. Kaneko***
- 16:20 – 95.** Environmentally degradable bio-based plastics from renewable itaconic acid and their composites with montmorillonite. **M. Ali***, N. Tandon, S. TATEYAMA, T. Kaneko
- 16:40 – 96.** Development of high thermoresistance and transparent polyurea films bioderived from 4-aminocinnamic acid. **Y. Ibuki***, S. TATEYAMA, T. Kaneko

Hawaii Convention Center
323B

Polymer Gels as Advanced Soft Materials (#83)

- Organized by:* R. Yoshida, T. Miyata, F. Winnik, J. Alzienberg
Presiding: F. Winnik, R. Yoshida
- 13:00 – 97.** Self-healing hydrogels from bilayer membrane. **J. Gong***
- 13:30 – 98.** Vitrimers: Insoluble and reshaping chemically crosslinked networks. **F. Tournilhac***
- 14:00 – 99.** Highly stretchable, mechanically tough, zwitterionic nanocomposite gels with controlled thermosensitivities and unique swelling and self-healing behaviors. **K. Haraguchi***
- 14:30 – 100.** One-step preparation of thermo/photo-sensitive nanogels and their use as stabilizers of Pickering high internal phase emulsions. **F. Winnik**, x. zhang
- 14:50** Break
- 15:00 – 101.** Hollow adaptive microgels. **W. Richtering***
- 15:30 – 102.** Designing microgels for hemostasis. N. Welsch, A. Brown, T. Barker, **A. Lyon***

- 16:00 – 103.** Polymer gels formed from critical gelation cluster. **T. Sakai**, K. Hayashi, U. Chung
- 16:20 – 104.** Composite particle synthesis in the presence of hydrogel particles. **D. Suzuki***, C. Kobayashi, T. Watanabe
- 16:40 – 105.** Uniform anisotropic colloids: Fabrication, assembly, and packing. **J. Kim***

Hawaii Convention Center
326B

Simulation of Polymers (#110)

Organized by: Y. Masubuchi,
S. Shanbhag, V. Vao-soongnern, C. Baig
Presiding: N. Arai, Y. Masubuchi

- 13:00 – 106.** Can heterogeneity in amorphous polymers be envisioned using atomistic simulation?. **F. Godey**, **A. Soldera***
- 13:20 – 107.** Molecular dynamics study on star-shaped thermoresponsive polymers in aqueous solution. **S. Sato***, E. Terada, M. Jin, S. Mizutani
- 13:40 – 108.** Atomistic molecular dynamics simulations of structure and thermodynamic properties of asymmetric polyelectrolyte block copolymer micelle in salt-free aqueous solution. **R. Chockalingam**, U. Natarajan*
- 14:00 – 109.** Self-assembly of bottlebrush copolymers and their blends with homopolymers: A Monte Carlo simulation study. **D. Jo**, J. Huh*, K. Lee
- 14:20 – 110.** Amphiphilic diblock copolymer mediated assembly of nanoparticles in solutions. **R. Wang***, S. Ma*
- 14:40 – 111.** Modeling and simulation of surfactants and polymer systems – what can we learn from these?. F.C. Lim, L. Zhang, D.W. Cheong, **M.B. Sullivan***
- 15:00 – 112.** Self-assembly of Janus origomers into onion-like vesicles. **N. Arai***, K. Yasuoka, X.C. Zeng
- 15:20 – 113.** Large scale simulation of a thermoplastic elastomer with SCFT and coarse-grained MD. **T. Honda**
- 15:40 – 114.** Coarse-grained simulations of interfaces between grafted polyelectrolytes. **T. Kinjo***, H. Yoshida, H. Washizu
- 16:00 – 115.** Multiscale simulation of contraction and expansion polymer melt flow. **T. TANIGUCHI***, K. HARADA
- 16:20 – 116.** Modeling the drying process of polymer solutions. **M. Doi***

Hawaii Convention Center
324

Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112)

Organized by: M. Kamigaito, C. Hawker, G. Qiao, K. Wooley, E. Yashima
Presiding: H. Otsuka, K. Wooley

- 13:00 – 117.** Organocatalytic strategies to novel macromolecular architectures. **R. Waymouth***
- 13:30 – 118.** Carbon dioxide as a renewable C1 feedstock for polymer synthesis. **K. Nozaki***
- 14:00 – 119.** Stereoselective, chemoselective, and living coordination polymerization of renewable acrylic monomers. **E. Chen**
- 14:30 – 120.** Non-equilibrated supramolecular interactions. **T. Aida***
- 15:00 – 121.** Investigating new sources for and applications of cellulose nanocrystals. **S.J. Rowan***
- 15:30 – 122.** Molecular design of dynamic covalent polymers for sustainability. **H. Otsuka***
- 16:00 – 123.** Organocatalyzed synthesis of high-molecular-weight aliphatic polycarbonates. **D. Kuckling***, A. Reitz, J. Sun, R. Wilhelm
- 16:15 – 124.** Aliphatic polyester/polycarbonate triblock copolymers via one-pot, neat, organocatalytic ring opening polymerization for generation of self-assembled polymeric nanoparticles. **A.J. Myles***, K. Moffat, J. Wosnick, V. Farrugia

- 16:30 – 125.** Synthesis of well-defined 3-dimensional P3HT based star polymers by GRIM and ATRP. **K. Baek***
- 16:45 – 126.** Switchable enantioseparation based on helicity induction and memory effect in a polyacetylene bearing 2,2'-bibiphenol-derived pendants in the solid state. **K. Maeda***, K. Shimomura, T. Ikai, S. Kanoh, E. Yashima*

Hawaii Convention Center
323C

Characterization of Polymers and Polymer Assemblies in Solution (#172)

Organized by: T. Sato, T. Yoshizaki, T. Chang, J. Mays, C. Wu

- 13:00 – 127.** Interaction chromatography separation of polymers: Principle and applications. **T. Chang***
- 13:45 – 128.** Getting the most from cumulants analysis of dynamic light scattering data... and getting it quickly. **P.S. Russo**, X. Zhang
- 14:30 – 129.** Comprehensive 2D analysis of poloxamers. **M.I. Malik***, S. Lee, T. Chang
- 15:00 – 130.** Characterization and fractionation of PS-*b*-PMMA diblock copolymer synthesized via click chemistry. **J. Park***, T. Chang, K. Lee, J. Kim
- 15:30 – 131.** Solubilization of 3-azido-1-propyne oligomers prepared by copper(I)-catalyzed azide–alkyne cycloaddition polymerization and characterization of the soluble oligomers in dilute solution. **A. Hashidzume***, A. Mori, S. Nakano, T. Nakamura, T. Sato
- 16:00 – 132.** Functional oligomeric fluids: Characterization challenges. **A.O. Patil***
- 16:30 – 133.** Reason for the high solubility of chemically modified poly(vinyl alcohol)s in aqueous solution. **T. Shikata***

Hawaii Convention Center
325A

Functional Materials Based on Organic-inorganic Hybrid Polymers (#221)

Organized by: K. Naka, F. Jaekle, C. Ha, J. Ohshita
Presiding: C. Ha, F. Jaekle, K. Naka, J. Ohshita

- 13:00 – 134.** Synthesis of element block polymers based on T8-caged silsesquioxanes. **K. Naka**
- 13:20 – 135.** Polymerizations with elemental sulfur: Novel inorganic polymers for energy, sustainability, and defense. **J. Pyun***
- 13:40 – 136.** Self-healing properties of photocrosslinked hybrids thin films using thiol-containing polysilsesquioxane. **K. Matsukawa***, K. Nishio, I. Urano, K. Mitamura, N. Nishioka, T. Koga, N. Higashi, S. Watase

14:00 – 137. Metallocenium polymers: From chemoselective synthesis to biomedical application. **C. Tang**

- 14:20 – 138.** Hybrid network polymer films of multifunctional cyclosiloxane building blocks. **M. Mitsuishi**, A. Demirci, Y. Liu, S. Yamamoto, J. Matsui, T. Miyashita

14:40 Break

- 14:50 – 139.** Chitosan based hybrid nanomaterials. **C. Ha**

- 15:10 – 140.** Hybrid polyurethane surface modification: Impact of nanosurface and mesosurface modification. **K.J. Wynne***, S. Chakrabarty, S. Nair, W. Zhang, V. Yadavalli

15:30 – 141. Preparation of graphene quantum dots and their chemical functionalization by Cu(II)-catalyzed Huisgen cycloaddition reaction. **R. Sekiya***, Y. Uemura, K. Suzuki, T. Haino

- 15:45 – 142.** CO₂-responsive magnetic mesoporous silica nanoparticles. **J. Guo**, **J. Yuan***

- 16:00 – 143.** Synthesis and characterization of self-organized N-heteroacene-based materials. **K. Isoda***

- 16:15 – 144.** Layer-by-layer assembly of a self-healing anticorrosion coating on magnesium alloy. **F. Fan**, J. Szpunar

- 16:30 – 145.** Dynamic cross-linking of POSS-containing polymers mediated by fluoride ion. **K. Tsuchiya**, H. Arai, Y. Ishida, A. Kameyama
- 16:45 – 146.** Polymer-grafted porous coordination nanocages. **N. Hosono***, R. Matsuda, S. Kitagawa

Hawaii Convention Center
327

Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281)

Organized by: M. Cunningham, M. Sawamoto, P. Chamapgne, J. Rawlins
Presiding: M. Cunningham, J. Rawlins

13:00 Opening Remarks - 5 mins

- 13:05 – 147.** Lipid based polymers: A bio-refinery approach enabled by structure function fundamentals. **S. Narine***

- 13:35 – 148.** Renewable monomers and polymers obtained via sustainable chemistry. **M. Meier**

- 14:05 – 149.** Enzymatically synthesized functional polyesters from renewable resources. **M. Bilal**, T. Naolou, A. Njau , J. Kressler

- 14:25 – 150.** Synthesis of functional poly-pentadecalactone copolymers by ring-opening polymerisation. **A.P. Dove**, J. Wilson

- 14:45 – 151.** Polymerization of biosourced myrcene using neodymium based catalysts. **R. Diaz de Leon***

- 15:05 – 152.** Synthesis of polyphenenamer and poly(vinyl alcohol) using phase separable PIB second generation Hoveyda-Grubbs catalyst. **M. Al-Hashimi***, R. Tuba*, H.S. Bazzi*, R.H. Grubbs*

- 15:25 – 153.** Design and synthesis of polyphosphoester-based multifunctional nanocarriers aimed for biomedical applications. **P. Ni***

- 15:55 – 154.** Crystalline nanocellulose functional and polymer grafting via surface initiated living radical polymerization. **J. Arredondo**, O. Garcia-Valdez, P. Champagne*, **M. Cunningham**

- 16:15 – 155.** Comparing surface esterification methods of cellulose nanocrystals for improved hydrophobicity. **S. Peng***, R. Moon, J. Youngblood

- 16:35 – 156.** Cellulose nanocrystal: A natural polymer to protect the functionality of active beads and edible coating. **m. lacroix***

Hawaii Convention Center
323A

Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319)

Organized by: X. Zhang, Q. Guo, W. Qin, T. Hu, K. Ramasamy
Presiding: T. Hu

- 13:00 – 157.** Synergistic catalysis of Fe based bimetallic catalysts for hydrode-oxygenation of lignin derived compounds. **Y. Hong**, A.J. Hensley, H. Zhang, J. Sun, A. Karim, M. Gu, M. Engelhard, J. McEwen, **Y. Wang***

- 13:25 – 158.** Reductive silylation of lignin: A route to oligomers and green composites. **M.A. Brook***, J. Zhang

* Principle Author

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13:45 – 159. Development of new functional materials using a metabolic intermediate of lignin, 2-pyrone-4,6-dicarboxylic acid. **H. Ogata**, Y. Otsuka, M. Nakamura

14:05 Break

14:15 – 160. Selective conversion of native lignin to aromatic dimer derivatives.

H. Nonaka, R. Yamamoto, M. Funao

14:35 – 161. Catalytic oxidation of bio refinery lignin to value added platform chemicals. **R. Ma**, X. Zhang*, M. Guo

14:55 – 162. Depolymerization of lignin into simple aromatics via Ni/HZSM-5 in an aqueous environment. **R. Barton***, N. Escalona, H. Lamb, S. Park, S. Peretti

15:15 – 163. Study on the mechanism of the pyrolysis of lignin model dimers by in situ FTIR. **H. Cheng**, S. Wu*

15:35 – 164. Demethylation of lignin-model aromatics over carbon-supported ruthenium-manganese catalyst.

Y. Nakagawa, M. Ishikawa, M. Tamura, K. Tomishige*

15:55 – 165. Lignin hydrogenolysis over Ni-based catalysts: Understanding the catalytic activity. **N. Yan***

Hawaii Convention Center
326A

Polymers for Energy and Optoelectronic Devices (#361)

Organized by: K. Oyaizu, R. Advincula, D. Choi

Presiding: D.H. Choi, K. Oyaizu

13:00 – 166. Novel conjugated polymer as both cathode and anode interlayers for inverted organic photovoltaics. **W. Wang**, Q. Zhang, D. Liaw, Y. Tai*

13:15 – 167. Triplet state formation in polymerfullerene photovoltaic blends.

F. Laqua*

13:30 – 168. Triplet state generation in photovoltaic blends of low-bandgap DPP-type copolymers and PC₇₁BM probed by transient absorption spectroscopy.

J.R. Ochsmann, D. Chandran, K. Lee,

F. Laqua*, M. Turbiez

13:45 – 169. Interplay between polymer donor and fullerene acceptor in bulk-heterojunction solar cells. **P.M. Beaujuge***

14:00 – 170. Improved stability for light soaking in efficient crystalline-Si/3,4-poly(ethylenedioxythiophene) (PEDOT) heterojunction solar cells. **H. Shirai***, Q. Liu*, R. Ishikawa, K. Ueno

14:15 – 171. Broadening the light absorption of P3HT derivatives using porphyrins: Noncovalent vs. covalent attachment.

M. Chevrier, S. Richeter, A. Mehdi, O. Coulombe, R. Lazzaroni, P.G. Dubois, S. Clement

14:30 Break

14:40 – 172. Photoprecursor approach towards efficient solution-processed organic solar cells. **M. Suzuki**, Y. Yamaguchi, K. Nakayama*, H. Yamada*

15:10 – 173. Polymer/dye composites for potential cost effective and high efficiency optoelectronic applications.

S. SUN*, D. Wang

15:25 – 174. PBDT[2FJT], the secrets of a wide band-gap polymer with 7% PCE.

J. Gorenflo, D.W. Gehrig, A. Paulke, J. Wolf, D. Neher, P.M. Beaujuge, F. Laqua

15:40 – 175. Effect of side chain volume of conjugated polymers on polymer:PCBM morphology and organic solar cell properties. **H. Son***

15:55 – 176. Polymeric interfacial engineering of the electrode for high performance solar cells. Y. Song, L. Yan, Y. Zhou*, B. Song*

16:10 – 177. Effective electron and hole extraction using novel polymeric materials in perovskite solar cells. **T. Park**, S. Song, G. Kim

16:25 – 178. Conjugated polyelectrolyte hole transport layer for inverted-type perovskite solar cells. H. Choi, C. Mai, H. Kim, J. Jeong, S. Song, G. Bazan, J. Kim*, A.J. Heeger

Wednesday Morning

Hawaii Convention Center
Halls I, II, III

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madsen, K. Saalwachter, Y. Yao, J. Battiste

Poster Session

10:00 – 12:00

179. Fast chain flips in mixed n-alkanes: Implications for polyethylene.

K.J. Fritzsching, Y. Marciano, K. Schmidt-Rohr*

180. Investigating ion transport and dynamics in a crosslinked polymer-gel lithium conductor. **B.E. Kidd**, S. Forbey, F.W. Steuber, R.B. Moore, L.A. Madsen*

181. Differentiating molecular and morphological effects on transport in an ionic polymer membrane. **M. Goswami***, L.A. Madsen

182. Measuring tunable anisotropy and ion transport in conductive, rigid, and thermally stable ion gels. **Y. Wang**, Y. Chen, J. Gao, H. Yoon, L. Jin, M. Forsyth, T. Dingemans, L.A. Madsen

183. Characterization of polymer microstructure and reaction mechanism by hyperpolarized NMR. **C. Chen**, C. Hilti

184. Monomer sequence in the poly(methyl methacrylate-co-benzyl methacrylate)s prepared by various polymer reactions of poly(benzyl methacrylate). **Y. Nakanishi**, Y. Hsu, T. Okubo, M. Oshimura, T. Hirano, K. Ute

185. Analysis of stereoregularity in poly(lactic acid) by solution NMR. **K. Suganuma**, H.N. Cheng, M. Oshimura, T. Hirano, K. Ute, T. ASAKURA

186. Monomer sequence in the poly(methyl methacrylate-co-benzyl methacrylate)s prepared by stepwise esterification of isotactic poly(methacrylic acid).

D. Yokota, Y. Nakanishi, M. Nagahama, T. Hirano, K. Ute

187. Magnetically oriented structures and gas transport properties of liquid crystalline polyesters with various higher-order structures by means of NMR methods.

R. Ishigami*

188. NMR of the gas in polyimides with different glassy states prepared by physical treatments. **M. Fujita***

189. Segmental motions in the noncrystalline domains of polyethylene. **W. Hu***, N. Patil

190. Chain dynamics in polymer crystalline region as investigated by solid state NMR. **W. Chen**, T. Miyoshi

191. Spin-spin relaxation time as a novel parameter for the quantitative evaluation of the degradation of rubber seals.

K. Numata*, H. Kurokawa, S. Sekine, Y. Nakazawa, A. Asano

192. Dynamics of water and protons in swollen polymer electrolyte membranes: Insight into proton transfer mechanism in fuel cells. **H. Kim**, O. Han

193. Inverse Laplace transform and principal component analysis of T_2 decays of polyisoprene rubbers filled with carbon black. **M. Tsunomura**, A. Asano*, T. Ohkubo, K. Okushita

194. Characterization of local pre-stretching in sequentially cross-linked polymer networks by NMR. **W. Chasse**, P. Millereau, V. Litvinov, C. Creton, A. Kentgens

195. ¹H-NMR investigations of semicrystalline polymers: Effects of preparation and molecular weight. **R. Kurz***

196. Determination of molecular dimension and trajectory of polymer chains embedded in single crystals. **Y. Hong**, T. Miyoshi

197. Topological and crystallization studies of well-defined PEG-networks.

M. Samiullah, D. Reichert*, T. Zinkevich, J. Kressler

198. Characterization of kerogen and source rock maturation using solid-state NMR spectroscopy. **A. Clough***, J. Sigle, J.L. White

199. Effects of temperature and pressure on the structure of ethylene- vinyl acetate copolymer (EVA). **R. Kuwahara**, N. Ogawa, R. Tomita, M. Nishino, Y. Kawakami, Y. Kawano, Y. Suzuki, M. Konno, . Nakajima, T. Takeda, K. Ishigami, H. Uehara, T. Yamane*

200. Characterization of a polymer complex of poly (allyl amine) and poly(acrylic acid) by solid NMR. **Y. Morozumi**, S. Maeda*

201. Characterization of polymer complex of poly(allylamine hydrochloride) and carboxymethyl cellulose sodium salt by solid NMR. **T. Kawaguchi**, S. Maeda*

202. Structural analysis of metal depositing polyamides for the novel wearable device. **T. Hashimoto**, Y. Tahara, M. Sano, T.M. Chang, M. Sone, H. Kuros

203. NMR studies for the development of tissue-engineering biomaterials based on silk fibroin and polyurethane.

C.T. Nakazawa, A. Higuchi, A. Asano, T. Kameda, Y. Nakazawa*

204. Improvement of *Bombyx mori* silk fibroin membranes with glycerin and NMR characterization. **T. Endo**, M. HIRAYAMA, M. Endo, T. ASAKURA*

205. Structure of *Samia cynthia ricini* silk fibroin with polyalanine sequences studied by solution and solid state NMR.

Y. Suzuki, S. Kawanishi, A. Aoki, H. Saito, T. ASAKURA*

206. Characterization of a polymer complex of poly (allyl amine) and poly (γ -glutamic acid) by solid NMR. **T. Kakishita**, S. Maeda*

207. Higher-ordered structure and gas transport properties of poly (γ -benzyl-L-glutamate) studied by NMR. **H. Yoshimizu***

Hawaii Convention Center

325B

Synthetic Biopolymers (#37)

Organized by: T. Deming, Z. Li, T. Kaneko

Presiding: T. Deming, T. Kaneko, Z. Li

8:00 Introductory Remarks

8:05 – 208. Hyperbranched biopolymers synthesized from amino acids. **Y. Li***

8:40 – 209. Polypeptoid polymers: Recent discoveries in the development of functional peptidomimetic polymers.

D. Zhang

9:15 – 210. Design of polypeptide and/or polysaccharide based copolymer self-assembled biomaterials.

S. LeCommandoux

9:50 Break

10:05 – 211. Synthesis and applications of responsive and functional polypeptides.

T. Deming*

10:40 – 212. Thermal and oxidation responsive polypeptide materials. **Z. Li***

11:00 – 213. Re-examination of amino acid NCA polymerization 64: Preparation of monodispersed high molecular weight polypeptides by the primary amine initiated polymerization of amino acid N-carboxy anhydride. **H. Kanazawa**, A. Inada

11:20 – 214. RAFT polymerization of polyphenol-inspired antioxidant polymers.

H. Ejima, Z. Kan, N. Yoshie

11:40 – 215. Controlled/living polymerization of naturally occurring terpenes.

K. Satoh*, M. Kamigaito

Hawaii Convention Center

323B

Polymer Gels as Advanced Soft Materials (#83)

Organized by: R. Yoshida, T. Miyata, F. Winnik, J. Alzenberg

Presiding: J. Alzenberg, T. Miyata

8:00 – 216. Photohealable materials based on photoreversible sol-gel transition of a triblock copolymer in an ionic liquid.

M. Watanabe*

8:30 – 217. Transforming the nanostructure of aqueous block ionomer gels for use in organic photovoltaics.

R.J. Spontak, H.A. Al-Mohsin, K.P. Mineart

9:00 – 218. Stimuli-responsively porating gels. **N. Kuriakose**, J. Texter*

9:20 – 219. Multifunctional polymer hydrogel-based hybrid membranes with stimuli-responsive properties. **M. Ulbricht***, M. Gajda, X. Lin, H. Ohashi

9:40 – 220. Stimuli responsive polymer-based sensors, muscles, and drug delivery platforms. **M.J. Serpe***

10:00 Break

10:10 – 221. Injectable purine-based sponges as a potential therapy to target remyelination post-spinal cord injuries. M. Mekhai, G. Almazan, **M. Tabrizian***

10:40 – 222. Synthetic gel based approach toward "electronics-free" artificial pancreas. **A. Matsumoto***, T. Ishii, H. Matsumoto, T. Suganami, M. Tanaka, Y. Ogawa, K. Kataoka, Y. Miyahara

11:00 – 223. Electrically induced controlled release from biopolymer capsules.

A. Gargava, R. Ponte, R. Ragunathan, S.R. Raghavan*

11:20 – 224. Photofabrication of 2.5-dimensional microstructures composed of hydrogel sheet. **K. Sumaru***, T. Takagi, T. Satoh, T. Kanamori

11:40 – 225. Thermoresponsive polymer brush possessing cationic group for purification of human bone marrow derived mesenchymal stem cell. **K. Nagase***, Y. Hatakeyama, T. Shimizu, K. Matsura, M. Yamato, N. Takeda, T. Okano

Hawaii Convention Center
Halls I, II, III

Simulation of Polymers (#110)

Organized by: Y. Masubuchi, S. Shanbhag, V. Vao-soongnern, C. Baig

Poster Session

10:00 – 12:00

226. Molecular dynamics simulations of concentration effect on conformations, hydrogen bond dynamics, and translational diffusion of poly(methacrylic acid) in salt-free aqueous solution. **R. Chockalingam**, U. Natarajan*

227. Molecular simulation of photon interaction with linear oligomers. **K. Narushima**

228. Dissipative particle dynamics simulations for self-assembly of polymer in vesicle. **Y. Yoshimoto***, N. Ara

229. Study of the adsorption of the cytochrome c on the graphene: Using molecular dynamics simulation. **X. Li**

230. Carrier generation mechanism in organic solar cells. **K. Narushima***, M. Takasaki

231. Dissipative particle dynamics simulation for morphology of telechelic star polymer solution: Effect of shape of polymer.

N. Nishida*, N. Ara

232. Dissipative particle dynamics simulation for self-assembly structure and rheological property of Janus nanoparticles solution in nanotubes. **Y. Kobayashi***, N. Ara

233. Comparison of viscoelastic response function between a united-atom model of polyethylene and the Kremer-Grest model. **R. NISHIMURA**, K. TAKAHASHI, K. Yasuoka, Y. Masubuchi

234. Molecular simulations for segmental motions of polymer chains. **K. Sasaoka**, T. Koga

* Principle Author

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<http://pacificchem.org/onlineprogram>

235. Computer simulation of dynamics of phase ordering of hydrogen-bonding supramolecular block copolymers.
R. Arimura*, T. Koga

Hawaii Convention Center
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Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112)

Organized by: M. Kamigaito, C. Hawker, G. Qiao, K. Wooley, E. Yashima
Presiding: T. Choi, E. Yashima

8:00 – 236. Increasing 3D supramolecular order by decreasing molecular order.
V. Percec*

8:30 – 237. Sustainable and degradable polymers from glucose and castor oil.
T.M. Reineke

9:00 – 238. Olefin metathesis and alkyne polymerization.
T. Choi*

9:30 – 239. Review for thermoreversible polymers consisting of multiple hydrogen bonds (MHB) and the pairs of Diels-Alder reaction.
K. Yamauchi*, D. Yamamoto, M. Yokoo, T.E. Long

10:00 – 240. Stereospecific polymerization and chiroptical properties of vinyl aromatics.
X. Wan*

10:30 – 241. Chirality transfer in chiral block copolymers.
R. Ho

11:00 – 242. Functional nanospace macromolecules via precision crosslinking and association technologies of polymer chains.
T. Terashima, M. Sawamoto

11:15 – 243. Precise synthesis of thermally curable hyperbranched polymers and their application to solvent-free adhesive materials.
E. Sato*, I. Uehara, T. Nishiyama, A. Matsumoto, H. Horibe

11:30 – 244. Remote stereocontrol of dynamic chiral structures.
N. Usaka*, F. Mamiya, E. Yashima

11:45 – 245. Enantioselective synthesis of chiral polymer from racemic monomer through the click polymerization directed by the circularly polarized light.
G. Zou*

Hawaii Convention Center
323C

Characterization of Polymers and Polymer Assemblies in Solution (#172)

Organized by: T. Sato, T. Yoshizaki, T. Chang, J. Mays, C. Wu

8:00 – 246. Cryo-electron tomography study of complex compartmentalized nanostructures.
A.H. Mueller*, T.I. Loebling, A.H. Groeschel, J. Haataja, C.V. Synatschke, F.H. Schacher

8:45 – 247. Characterizing polymeric micelles employed for DDS combining SAXS and FFF.
K. Sakurai, Y. Sanada, I. Akiba

9:15 – 248. Association behavior of bovine serum albumin with the PEO-PPO multiblock copolymer in water.
K. Rikiyama*, Y. Katsumoto

9:45 – 249. Characterization of complexes formed by mixing aqueous solutions of polymethacrylic acid and a homopolymer or block copolymer of 2-ethyl-2-oxazoline.
Y. Matsuda*, M. Kikuchi, A. Takahara, S. Tasaka

10:30 – 250. Intermolecular interaction and self-assembly in aqueous solutions of a mixture of anionic-neutral and cationic-neutral block copolymers.
R. Takahashi, T. Sato, K. Terao, S. Yusa

11:00 – 251. Two aggregation processes of thermo-responsive PEO-PPO multiblock copolymer in the aqueous solution.
T. Horie*, S. Kondo, T. Sakai, Y. Katsumoto

11:30 – 252. Overview of self-assemblies formed by amphiphilic block, random, and alternating copolymers.
T. Sato*

11:55 Closing Remarks

Hawaii Convention Center
325A

Functional Materials Based on Organic-inorganic Hybrid Polymers (#221)

Organized by: K. Naka, F. Jaekle, C. Ha, J. Ohshita
Presiding: C. Ha, F. Jaekle, K. Naka, J. Ohshita, I. Tomita

8:00 – 253. Enhancement of photoluminescence and electroluminescence of samarium complex by polysilsesquioxane.
S. Watase*, T. Yamashita, Y. Hasegawa, K. Mitamura, T. Koga, N. Higashi, K. Matsukawa

8:15 – 254. Monitoring the formation of fluorescent micelles from crystallization driven self-assembly using STED and TEM.
E. Leitao, I. Manners

8:30 – 255. Attempted synthesis of functional materials using metalladithiolene complexes.
S. Tsukada, T. Sagawa, H. Sato, T. Gunji*

8:45 – 256. Synthesis and optical properties of cyclic and acyclic poly(germylethylene-ethynylene) materials.
H. Tanimoto*, T. Nagao, T. Fujiwara, K. Tanaka, T. Kakuta, Y. Chuo*, K. Kakuchi*

9:00 – 257. π -Conjugated polymers containing versatile elements-blocks.
I. Tomita*, Y. Matsumura, Y. Komatsuzaki, H. Nishiyama, S. Inagi

9:20 – 258. Sol-gel silica nanoparticals and their application to functional organic/inorganic hybrid coating.
D. Lee, S. Han, D. Kang

9:40 Break
9:50 – 259. Functional soft materials from the self-assembly of block copolymers containing main group elements and metals.
I. Manners*

10:20 – 260. Ionic liquid/boron compound binary electrolytes for lithium ion secondary batteries.
N. Matsumi

10:40 – 261. Preparation and applications of disilanobiphenole and -biphenyl as new silicon-bridged chromophores.
J. Ohshita

11:00 – 262. Organic/inorganic hybrid nanostructures for organic electronic devices with polymer semiconductors.
C. Lee, W. Lee, J. Seo, H. Kim, **Y. Kim***

11:20 – 263. Well-defined "N-type" organic electronic materials.
D.S. Seferos

11:40 – 264. Synthesis of ferrocene-containing polytriazoles by metal-free click polymerization.
A. Qin*, B. Tang

Hawaii Convention Center
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Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281)

Organized by: M. Cunningham, M. Sawamoto, P. Chamapgne, J. Rawlins
Presiding: M. Sawamoto

8:00 Open Remarks

8:05 – 265. Multifunctional nanoworms and nanorods and functional membranes.
M. Monteiro

8:35 – 266. Biosourced polymer nanocomposites: high performance materials for durable applications.
P.G. Dubois*, M. Maruri, J. Raquez, L. Bonnaud, J. Odent

9:05 – 267. Novel efficient ligation reactions for polymer chemistry.
S. Perrier*

9:35 – 268. Chitosan-based flame retardant multilayer nanocoatings.
J. Grunlan*, T. Guin, M. Leistner

9:55 – 269. Synthesis and application of multifunctional nitrile N-oxides.
H. Sogawa*, S. Monjihama, T. Takata

10:15 – 270. Conceptualizing sustainable thermoplastic elastomers from hydrocarbon-rich biomass.
C. Tang

10:45 – 271. Hybrid materials based on nanoscopic cellulose and well-defined polymers.
E. Malmstrom*, A. Carlmark

11:15 – 272. Modification of chitosan via nitroxide-mediated polymerization and grafting from approach in homogeneous media.
O. Garcia-Valdez, A. Darabi, R. Champagne Hartley, E. Saldivar-Guerra, **P. Champagne***, M. Cunningham

11:35 – 273. Alginate-based amphiphilic graft copolymer prepared via living radical polymerization.
V. Kapishon, R. Whitney, P. Champagne, R.J. Neufeld, **M. Cunningham***

Hawaii Convention Center
328A

Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319)

Organized by: X. Zhang, Q. Guo, W. Qin, Y. Hu, K. Ramasamy
Presiding: Q. GUO, X. Zhang

8:00 – 274. Studying bacterial lignin degradation in soil actinomycetes.
M.C. Chang*

8:20 – 275. Delignification of rice straw by *Trametes hirsuta* and *Myrothecium roridum* and comparison of saccharification yields with dilute acid pretreatment.
D. Carrier*, A. Arora, K. Rajan

8:40 – 276. Biodegradable lignin composites from biorefinery plant.
I. liu

9:00 – 277. Biocatalytic routes of lignin to high value chemicals.
M. Tu*

9:20 – 278. Biomimetic Fenton catalyzed lignin depolymerization to aromatics and low molecular chemicals.
z. tong*, j. zeng, C. Yoo, f. wang, x. pan, w. Vermerris

9:40 break
9:50 – 279. Hydrothermal decomposition of Cunninghamia lanceolata enzymatic/mild acidolysis lignin at different temperature in subcritical water.
Y. Zhao, X. Li, S. Wu*, Y. Li

10:10 – 280. Fungal demethylation of Kraft lignin for polymer applications.
L. Christopher, B. Venkatesagowda, L. Maleki, R. Dekker

10:30 – 281. Lignin modification by ionic liquid.
M. Nejad*, M. Arefmanesh, E. Master

10:50 – 282. Low temperature hydrothermal decomposition of a lignin dimer model compound.
D. Liu, J. Sun, E. Nagel, C. yuhe, z. Gu, **C. Zhang***

11:10 – 283. Lignin conversion to value-added products.
M.A. Litga*, S. Lee

11:35 – 284. Overview of the main features of the LignoForte SystemTM, the lignin product and emerging high-value applications.
M. Paleologou*, L. Kouisni, K. Maki, B. Richardson, Y. Zhang, M. Feng, P. Fatehi

Hawaii Convention Center
326A

Polymers for Energy and Optoelectronic Devices (#361)

Organized by: K. Oyaizu, R. Advincula, D. Choi
Presiding: R. Advincula, K. Oyaizu

8:00 – 285. Graphene/Polymer based templated electronic materials.
R. Advincula*

8:20 – 286. Out-of-plane structural and optical properties of solvent-treated PEDOT/PSS films.
K. Itoh, Y. Honma, N. Asano, T. Sasaki

8:35 – 287. Electrical conduction properties in oriented films of conductive polymer PEDOT/PSS.
Y. Honma, N. Asano, Y. Kato, K. Itoh, M. Guziak, T. Nishizaki, H. Masunaga, A. Fujiwara, T. Sasaki

8:50 – 288. Nanocrystallization process in acid-treated PEDOT/PSS films investigated by wide-angle X-ray diffraction.
N. Asano, Y. Honma, Y. Kato, K. Itoh, H. Masunaga, A. Fujiwara, T. Sasaki

9:05 – 289. Controlling porosity of solution-deposited inherently conducting polymers to maximize electrochemical performance.
J.A. Irvin*, T. Cantu, J.R. Garcia, J. Frazer, T. Morgan, S. Vong

9:20 – 290. Whispering gallery mode photo-emission from π -conjugated polymer microspheres and efficient intersphere energy transfer.
S. Kushida*, D. Braam, T.D. Dao, S. Kosuke, H. Saito, S. Ishii, T. Nagao, J. Kuwabara, T. Kanbara, M. Kijima, A. Lorke, Y. Yamamoto
9:35 Break

9:45 – 291. Fine-controlled metal-assembling polymers for advanced nanomaterials.
K. Yamamoto

10:15 – 292. Dynamic covalent synthesis of conjugated ladder polymers.
L. Fang

10:30 – 293. Azza-Diels-Alder route to polyquinolines.
D.J. Dibble, M.J. Umerani, A. Mazaheri, Y.S. Park, J.W. Ziller, A.A. Gorodetsky

10:45 – 294. In-situ formation of conjugated polymers via vapor-phase polymerization for optoelectronic applications.
T. Suga*, H. Nishide

11:00 – 295. Polyether-based electrolyte blends with nano-ordered phase separated structure for novel antistatic materials.
Y. Kubota, Y. TOMINAGA

11:15 – 296. Fully organic multilayer nanocoatings with thermoelectric power factor that rivals inorganic tellurides.
J. Grunlan*, C. Yu

Hawaii Convention Center

Halls I, II, III

Macromolecular General Posters

10:00 – 12:00

Polymer Synthesis

297. Synthesis of graft copolymers and dendronized polymers by Cu-catalyzed multicomponent polymerization.
H. Kim, K. Bang, J. Lee, T. Choi*

298. Ethylene-propylene copolymerization initialized by V complexes.
H. Ren, Y. Yi, C. Li

299. Synthesis of helically chiral liquid crystalline polyphosphazenes.
M.L. Koerber*, C.M. Thiele

300. Lignin-b-PMMA micelles via reversible addition-fragmentation chain transfer polymerization.
M. Callari*, M. Stenzel, M. Hernandez-Guerrero

301. Novel radical initiation system consisted of halalkane/amine for free radical polymerizations of methyl acrylate, methyl methacrylate and styrene.
H. Tang*, C. Xu

302. Toward the synthesis of functionalized, helically-chiral polyisocyanites as transition-metal- or organocatalysts.
S. Otto, M. Reggelin

303. Synthesis and catalytic activity of palladium nanoparticles using phenylazomethine dendrimer as atom number controlling templates.
T. Kofuku, H. Kitazawa, K. Albrecht, W. Chun, T. Imaoka, K. Yamamoto

304. Controlled synthesis of novel poly(vinyl ether)-grafted poly(phenylacetylene)s by a combination of living coordination polymerization and living cationic polymerization.
S. Kawamura, J. MOTOGANAGI, M. MINODA

305. Novel molecular brush grafted poly(phenylene vinylene) (PPV) and poly(phenylene ethynylene) (PPE).
M. Damavandi

*** Principle Author**

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306. Synthesis of a water-soluble polypeptide containing thioester bonds on its side chains and dynamic exchange reaction using the thioesters. **S. URAI**, T. Oyama

Applications of Polymers

307. Development of the phosphorus and nitrogen containing flame retardant for value added cotton product. **B. Condon**, S. Chang

308. Analysis of fouling behavior of PVA-based anion-exchange membranes in electrodialysis processes. **R. Hironaga***, M. Higa

309. Study of the ability of phase transfer catalyst of the styrene based polymer having a hexaalkyl guanidinium salt. **S. Tanaka**, N. Iwasaki

310. Preparation and membrane characterization of a temperature-responsive anion exchange membrane. **T. Mizuno***, M. Higa

311. Production of Pickering emulsions stabilized by associative magnetic nanoparticles for recoverable emulsion flooding. **S. Choi***, T. YANG, J. Kim

312. Liquid crystals alignment properties of photopolymer with different photosensitive group. **J. Kang***, S. Yang, H. Song, **K. Choi**, S. Lee, G. Shin*

Polymer Characterization

313. Thermal decomposition of plastics at low temperature and ocean contamination generated from debris plastics. **K. Koizumi**, K. Amamiya, A. Okabe, D.M. Karl, K. Takatama, M. Nishimura, **K. Saido**

314. Pulse radiolysis studies on the early reactions of polystyrene derivative resists. **C. Wang***, Y. Hosaka, Y. Ito, A. Oshima, T. Kondoh, M. Washio, S. Tagawa

315. Characterization of ion exchange membranes prepared from poly (vinyl alcohol) based block copolymers. **M. Anno***, T. Mizuno, M. Higa

316. Stable helical phase in chiral block copolymers with high degree of chirality. **H. Wang**, Z. Fu, J. Lee, M. Li, J. Tsai, R. Ho

317. Clarification of the structural dependency of the inner microenvironments of poly(N-isopropylacrylamide) gels using a fluorescent probe technique. **D. Ito**, H. Itagaki

Polymer Processing

318. Electrospun nanofibre scaffolds for tissue engineering. **E.W. Chan***

319. Ordering and alignment in high molecular-weight block copolymer films by neutral solvent vapor annealing. **S. Park***, Y. Kim, **D. Ryu**

320. Purification of starting material, intermediates, and final products by recycling prep HPLC. **K. Tseng***, I. Hideto, T. Karasawa

321. Reactive extrusion of polyethylene terephthalate. **A. Ozdemir**

322. Ultra-high thermoresistant, transparent bio-polyimides from 4-aminocinnamate photodimer. **j. singh***, T. Kaneko, S. TATEYAMA, P. SUVANNASARA

323. Innovative green technique for preparing of flame retardant cotton. **S. Chang***, B. Condon, J. Smith

324. Toughening of epoxy resin by using cleavage of the covalent bonds between matrix and modifier during curing reaction. **T. Kaga***, T. Oyama

325. Miscibility enhancement of poly(vinyl-chloride)/polystyrene blend: Application as membrane for separation of benzene/cyclohexane mixture by pervaporation. **D.M. Aldhayan**

326. Polymer films having hierarchically ordered surface structure by a combination of nanoimprinting and surface-initiated controlled polymerization 1: Concept and examples using polymers bearing dithiobenzote or benzyl chloride residues. **M. MINODA***, T. Uemura, T. Matsumoto, M. Sumida, J. MOTOYANAGI

327. Polymer films having hierarchically ordered surface structure by a combination of nanoimprinting and surface-initiated controlled polymerization 2: Films made of polymers bearing photolinkable moieties and their surface properties. **T. Nohara***, T. Uemura, J. MOTOYANAGI, M. MINODA

Hydrigels

328. X-ray diffraction study on structural change of polymer hydrogels during dehydration. **R. Naohara**, K. Narita, Y. Okanoya, Y. Sekine, T. Ikeda-Fukazawa

329. Effect of side chain structure on dehydration process of polymer hydrogel. **Y. Tojima**, T. Ikeda-Fukazawa, Y. Sekine

330. Wholly π -conjugated organogels based on pyrene-containing oligo(*m*-phenylene ethynylene)s. **Y. Chen**, **H. Wang***, D. Zhang, Z. Li

331. Tough, thermoresponsive hydrogels. **J. Cubuk**, S. Rajaraman*, P. Cohn*, D. Shah, M. Jani

332. Water states in physically cross-linked nanogels. **J. Kodama**, Y. Sekine, K. Akiyoshi, T. Ikeda-Fukazawa

Polymers for Electronics and Photonics

333. Synthesis of red-fluorescent π -conjugated polymers via direct arylation and their π -stacked gel formation. **S. Hayashi**, T. Koizumi

334. Synthesis of π -conjugated polymers from cross-conjugated poly(2,3-diaryl[2]dendralene)s and their optical properties. **T. Koizumi***, A. Kameda, S. Hayashi

335. Facile method for making PEDOT/PSS conductive microparticle with magnetite (Fe_3O_4) using a microfluidic droplet devices. **S. Lee**, J. Yim, Y.S. Ko

336. Syndiotactic polystyrene films co-crystallized with organometallic complex and conductive polymer. **T. Sano***, T. Okabe, Y. Kuboyama, H. Itagaki

337. Synthesis and suspension rheology of hydrophobically modified associative nanoparticles. **T. YANG***, S. Choi, J. Kim

Polymers for Bio-applications

338. Water-soluble fluorescence-switching polymers for super-resolution bioimaging. **M. Zhu**

339. Cereal protein polymer properties on processing and cure within a totally bio-based adhesive system. **N. Hati***, W. Grigsby, J. Jin, N. Edmonds

340. Evaluation of the physical properties of funori adhesive to be used for cultural properties. **Y. Hara***, N. HAYAKAWA, T. HONDA

Wednesday Afternoon

Hawaii Convention Center
323B

Polymer Gels as Advanced Soft Materials (#83)

Organized by: R. Yoshida, T. Miyata, F. Winnik, J. Aizenberg

Presiding: J. Aizenberg, T. Miyata

13:00 – 341. Supramolecular gels in energy and medicine. **S. Stupp***

13:30 – 342. Macroscopic self-assembly through molecular recognition. **A. Harada***

14:00 – 343. Designs of target molecule-responsive gels with cyclodextrins and their smart properties. **T. Miyata***, A. Kawamura, T. Uragami

14:20 – 344. Biomolecule triggered shape transformations of hybrid hydrogels. **J. Athas***, C. Nguyen, B.C. Zarket, Z. Nie, S.R. Raghavan*

14:40 Break

14:50 – 345. Anisotropic hydrogels with magnetically oriented 2D electrolytes. **T. Aida***

15:20 – 346. Modeling the entrainment of self-oscillating gels to an applied, periodically varying force. **V. Yashin**, S. Levitan, **A. Balazs***

15:50 – 347. Spatiotemporal control of self-oscillating gel by uniformly aligned inorganic nano sheets. **Y. KIM***, Y. Ishida, Y. Ebina, T. Sasaki, R. Yoshida, T. Aida

16:10 – 348. Self-oscillating vesicles: Spontaneous cyclic changes of supramolecular structures formed by synthetic diblock copolymers. **R. Tamate***, T. Ueki, M. Shibayama, R. Yoshida

16:30 – 349. Functional hydrogels with a pinch of vanilla. **D. Kuckling***, Z. Chen, M. Ali, M. Roth, W. Birnbaum, M. Tiemann

Hawaii Convention Center
324

Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112)

Organized by: M. Kamigaito, C. Hawker, G. Qiao, K. Wooley, E. Yashima
Presiding: A. Almutairi, G.G. Qiao

13:00 – 350. Precise polymers and polymeric hybrids by ATRP. **K. Matyjaszewski**

13:30 – 351. Design and characterization of (polymer/ natural inorganic nanotube) assemblies. **A. Takahara**

14:00 – 352. Controlled polymerization in the formation of nanoscale thin films. **G.G. Qiao***

14:30 – 353. Stimuli-responsive polymers for patterning hydrogels. **A. Nelson**

15:00 – 354. Light-degradable polymers: Amplification strategies, response to new wavelengths, and application to a clinical challenge. **J. Olejniczak**, C. Carling, A. Garcia, V. Nguyen Huu, J. Luo, K. Zhang, **A. Almutairi**

15:30 – 355. Sterically protected nucleic acids for supramolecular assembly and in vivo delivery. **K. Zhang**, X. Lu, X. Tan, F. Jia, E. Watts

16:00 – 356. Mechanically responsive surfaces and interfaces via surface-initiated controlled radical polymerization. **H. Klok**

16:15 – 357. High fidelity IR 1D photonic crystals via brush polymer self-assembly. **R.J. Macfarlane***, R.H. Grubbs

16:30 – 358. Star polymer coatings for biocompatible interfaces. **T. Ando***, M. Totani, K. Terada, M. Kobayashi, M. Tanihara

16:45 – 359. Hollow polymer microspheres for targeted, responsive delivery. **G.J. Price***, E.G. Cradduck, E.K. Skinner

Hawaii Convention Center
323C

Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194)

Organized by: K. Tanaka, A. Crosby, S. Kim, K. Dalnoki-Veress
Presiding: M. Seo, K. Tanaka

13:00 – 360. Bicontinuous nanostructures via polymerization-induced microphase separation. **M. Seo***

13:30 – 361. Synthesis and characterization of cationic organoanion dendrimers. **C. Agatemo***, A.A. Abdelghani, B. Thabet, N. Etkin, R. Bissessur, A.S. Abd-El-Aziz

13:45 – 362. Repeatable adhesion system using proton-acceptable and donative polymer brushes. **M. Kobayashi***

14:00 – 363. Electrodeposition of metal oxides onto polymer surface. **M. Watanabe***, T. Shinagawa, S. Watase, T. Tamai, K. Matsukawa

14:15 – 364. Automatic vertical alignment of nematic liquid crystals by directly introducing giant surfactants. **K. JEONG***

14:30 – 365. Controlling nanocomposite hydrogel mechanics via bioinspired interfacial bond dynamics. **N. Holten-Andersen***

15:00 – 366. New aspects in tribological properties of concentrated polymer brushes with large thicknesses. **Y. Tsuji***, S. Hsu, D. Ishibashi, K. Ohno

15:30 – 367. Lubrication properties of ionic liquid polymer brushes combined with molecularly smooth sheets. **H. Arafune**, T. Kamijo, T. Morinaga, T. Sato*

15:45 – 368. Self-healing of a cross-linked polymer with dynamic covalent linkages at ambient temperature. **K. Imato**, A. Takahara*, H. Otsuka*

16:00 – 369. Enzymatic synthesis of reactive cellulose nanosheets and their functionalization through click chemistry. **Y. Yataka**, T. Sawada, T. Serizawa*

16:15 – 370. Control of interfacial structure and dynamics of vinyl polymers for bio-applications. **Y. Oda***

Hawaii Convention Center
325A

Functional Materials Based on Organic-inorganic Hybrid Polymers (#221)

Organized by: K. Naka, F. Jaekle, C. Ha, J. Ohshita
Presiding: C. Ha, F. Jaekle, K. Naka, J. Ohshita

13:00 – 371. Conversion of biowaste silica to alkoxysilanes without using silicon. **R.M. Laine***, J.C. Furgal, V. Popova

13:20 – 372. Advanced research in the fully return-to-nature polymer. **S. Kim**

13:40 – 373. Facile preparation of ionic cyclotriphosphazanes using superacid catalysts. **Y. Kaneko***

14:00 – 374. Mixing metals and macromolecules: Hybrid cobalt-block copolymer materials. **R.B. Grubbs***

14:20 – 375. Hierarchical structure design of necklace shaped inorganic polymer networks works alternately bearing a POSS cage and siloxane chains. **M. Kunitake**

14:40 – 376. Influences of anti-corrosive sol-gel precursors containing amino-quinone functional groups on the protection of the metal substrates against the corrosion. **M. Han***

15:00 – 377. Amphiphilic polyhedral silsesquioxanes (POSS) for self-assemble and ion conductive materials. **J. Matsui***, M. Takeda, K. Kuroiwa, T. Miyashita, M. Mitsuishi

15:20 Break

15:25 – 378. Silicon and tin containing block copolymers for high resolution lithographic applications. **C.G. Willson***, C.J. Ellison, M. Maher, G. Blachut, S. Sirard, Y. Asano, W. Durand, M. Carlson, K. Mori

15:45 – 379. Self-organized hybrid polymer films for hierarchical porous structures. **T. Hayakawa***, K. Okuhara, R. Maeda, Y. Kushima, K. Azuma, Y. Tanaka

16:00 – 380. Hybrids organic/inorganic materials in chromatographic separations. **B. Murithi**, K. Wyndham, N. Lawrence, D. Walsh, P. Irneta, B. Alden, T. Walter

16:15 – 381. Polysaccharide derivatives with near-infrared dyes for optical and photoacoustic tumor imaging. **K. Miki***, K. Ohe*

16:30 – 382. Supramolecular control of optical and magnetic properties in functional metal complexes with diblock copoly-peptide amphiphiles. **K. Kuroiwa***

16:45 – 383. Polystyrene-silica nanocomposites with well-controlled nanostructures provided from perhydroxypolysilazane. **R. Saito***, H. Hashimoto, H. Nakaseko

* Principle Author

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Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281)

Organized by: M. Cunningham,
M. Sawamoto, P. Chamapgne,
J. Rawlins
Presiding: M. Cunningham, J. Rawlins

13:00 – 384. Development of smart polymer applications for innovative separation of natural homologues. **S. Zhu***, W. Wang
13:30 – 385. Living copolymerization of isobutylene and alkoxycarbene for block copolymer synthesis. **J.E. Puskas**,
A.L. Gergely

14:00 – 386. Radical ring-opening polymerization of cyclic ketene acetal revisited: An experimental and theoretical study. A. Tardy, C. Lefay, D. Gimenes,
Y. Guillaneuf*

14:20 – 387. Precision polymerization of renewable vinyl monomers for sustainable polymers. **M. Kamigaito***, K. Satoh
14:50 – 388. Design of catalysts for sustainable and precision syntheses of functional polymers. **M. Ouchi***

15:20 – 389. ATRP catalyst separation and recycling. X. Jiang, M. Ding, L. Zhang,
Z. Cheng*, X. Zhu

15:50 – 390. Passerini multicomponent polymerization as a green polymerization method for new polymer synthesis. **Z. Li**

16:20 – 391. Green route to biobased polyesters: Solvent-free thin film reactions for enzymatic polycondensations. **A. Pellis**,
L. Corici, V. Ferrario, E. Herrero Acero,
C. Ebert, G.M. Guebitz, L. Gardossi*
16:40 – 392. Co₂-triggered stimuli-responsive polymers for separations. Q. Zhang,
P. Liu, G. Yu, Y. Lu, **W. Wang***, B. Li,
S. Zhu

Hawaii Convention Center
323A

Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319)

Organized by: X. Zhang, Q. Guo, W. Qin,
T. Hu, K. Ramasamy
Presiding: X. Zhang

13:00 – 393. Pretreatment, can we achieve effective biomass hydrolysis without removing lignin? **J.N. Saddler***

13:25 – 394. Biobased epoxy nanocomposites and thermoplastics derived from lignin-based monomers.
M.M. Abu-Omar*, S. Zhao

13:45 – 395. Improving yield and deoxygenation of bio-oil produced by pyrolysis of mixtures of black liquor and selected additives. **A. van Heiningen***

14:05 – 396. Development of mechanoresponsive lignin hydrogels with self-healing properties. **D. Kai***, X. Loh

14:25 – 397. Thermally induced structural transformation of lignin during processing. **S. Rennecker***, M. Cho, W. Zhang,
N. Sathitsuksanoh, B. Simmons, F. Ko

14:45 – 398. Study on the mechanism of synthesis of lignin-phenol-urea-formaldehyde co-condensed adhesive synthesized under alkaline condition. S. Yang*,
T. Yuan*, **R. Sun***

15:05 break

15:15 – 399. Study on catalytic microwave pyrolysis lignin for production of aromatic hydrocarbon rich chemicals. **Q. Bu***

15:35 – 400. Characterization and optimization of alkaline wet oxidation of biorefinery lignin obtained from pretreated forest slash. **K. Srinivas**, F.d. Oliveira, P. Teller,
A.R. Goncalves, B.K. Ahring*

15:55 – 401. Risks associated with producing and using lignin from acidic pretreatment of non-woods. **R.C. Francis***

16:15 – 402. Performance enhancement of lignin-based thermosets and polymer blends. **J. Xin***, X. Guo, **J. Zhang**

16:35 – 403. Influence of lignin degradation methods on the biorefinery lignin structure analysis. **X. Zhang**, Y. Matsumoto

Hawaii Convention Center
326A

Polymers for Energy and Optoelectronic Devices (#361)

Organized by: K. Oyaizu, R. Advincula,
D. Choi
Presiding: R. Advincula, K. Oyaizu

13:00 – 404. Polymer-based resistive non-volatile memory devices. **T. Lee***

13:30 – 405. Phthalocyanine-cored star-shaped polymers for the application in organic memory devices. **J. Aimi***, C. Lo, W. Chen

13:45 – 406. Polyfullerene electrodes for high power supercapacitors. **T.B. Schon**,
P.M. DiCarmine, D.S. Seferos*

14:00 – 407. TiO₂/polyaniline core/shell nanocomposite for high performance supercapacitor electrode. B. Patil, K. Jang, D. Kim, **H. Ahn***

14:15 – 408. Synthesis and reversible negative charge storage capability of an-thraquinone substituted poly(norbornene). **T. Kawai***, K. Oyaizu, H. Nishide

14:30 – 409. Biohydrogen production from sugary waste water for clean energy. **E. Dewi***, Z. Dwi Hastuti, C. Yeon Chu, U. Priyanto

14:45 Break

14:55 – 410. Poly(ethylene carbonate)-based composite electrolytes for all-solid-state lithium polymer batteries. **K. Kimura**, Y. TOMINAGA*

15:10 – 411. Superionic conductivity and high temperature stability of photopolymerized solid polymer electrolyte networks. **T. Kyu***

15:25 – 412. Rocking chair-type charge-discharge property of redox copolymers and polymer composites containing TEMPO and charge-neutralizing anion.

H. Tokue*, T. Murata, K. Oyaizu, H. Nishide

15:40 – 413. Redox-active polyimide-polyether block copolymers as electrode materials for lithium batteries. **G. Hernández**, N. Casado, R. Coste, D. Shamukaraj, L. Rubatat, M. Armand*, D. Mecerreyres*

15:55 – 414. Polymers with enhanced redox mediation capability for high performance energy storage devices. **K. Oyaizu***, H. Nishide

16:10 Closing Remarks

Wednesday Evening

Hawaii Convention Center
324

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English,
H. Kaji, S. Kawahara, A. Whittaker,
J. White, L. Madsen, K. Saalwachter,
Y. Yao, J. Battiste
Presiding: H. Cheng

19:00 Introductory Remarks

19:03 – 415. Polymeric MRI agents for disease detection: Advances and challenges. C. Zhang, K. Wang, H. Peng, s. puttik, T. Thurecht, S. Rose,
A. Whittaker*

19:42 – 416. Using NMR diffusometry and microimaging to probe soft materials from molecular to millimeter scales.
L.A. Madsen*

20:21 – 417. Solid state NMR of polymers: Ready to retire or forever young?
H.W. Spiess*

Hawaii Convention Center
Halls I, II, III

Synthetic Biopolymers (#37)

Organized by: T. Deming, Z. Li,
T. Kaneko

Poster Session

19:00 – 21:00

418. Re-examination of amino acid NCA polymerization 66: Preparation of monodispersed high molecular weight polypeptides by the polymerization of amino acid N-carboxy anhydride initiated by tertiary amine. H. Kanazawa, **Y. Kanazawa**, A. Inada

419. Synthesis of amylose-analogous heteropolysaccharides by phosphorylase-catalyzed enzymatic copolymerization. **R. Baba**, Y. Takata, K. Yamamoto, J. Kadokawa*

420. Photoswelling of poly(cinnamoyl ester)s with a zig-zag backbone. **S. Rawat***, T. Kaneko, K. Okeyoshi, S. TATEYAMA, k. yasaki

421. Accelerating the degradation and clearance of β -amyloid fibrils by a decapeptide inhibitor peptide. Q. Zhang, J. Liu, X. Hu, **W. Wang***, Z. Yuan*

422. Synthesis of poly(ω -methoxyalkyl acrylate)s and their blood compatibility evaluation. **M. Wakui**, S. Kobayashi, R. Satou, M. Tanaka*

423. Enzymatic synthesis of amphoteric polysaccharide materials. **Y. Takata**, K. Yamamoto, J. Kadokawa*

424. Effective saccharification of cellulosic biomass and ethanol fermentation. **A. Gulibusitan***, X. Liang, T. Uryu, T. Yoshida

425. Reactive gels and dispersions made with water-based extracts from canola meal. **A. Parker***, J. Marcinko, D. Parker

426. Synthesis of glycodendrimers with different branched numbers for DDS purpose. **S. Han***

427. Enhancement of proton transport in an oriented polypeptide thin film. **S. Laakroekkhat**, Y. Nagao*, J. Matsui, T. Abe, H. Hiramatsu, H. Yamamoto, T. Miyashita

428. Cysteine derived cross-linker for an-ionic UV curing of epoxy resins. **M. Furutani**, S. Sato, K. Arimitsu*

Hawaii Convention Center
323B

Polymer Gels as Advanced Soft Materials (#83)

Organized by: R. Yoshida, T. Miyata,
F. Winnik, J. Alzienberg
Presiding: T. Miyata, R. Yoshida

19:00 – 429. Biomimetic growth of a pathologic biominerals in hydrogels. G. Mallam, **M. Tsianou***

19:20 – 430. Highly sensitive signaling molecularly imprinted nanocavity for biomarker protein prepared via post-imprinting in-cavity functionalization.

R. Horikawa, H. Sunayama, Y. Kitayama, T. Takeuchi*

19:40 – 431. Temperature-assisted assembly of monodisperse, covalently cross-linked, and degradable poly(N-isopropylacrylamide) microgels based on oligomeric precursors. D. Sivakumaran, E. Mueller, **T. Hoare***

20:00 – 432. Phase-separated thiol-epoxy-acrylate hybrid networks with controlled crosslink density synthesized by simultaneous thiol-acrylates and thiol-epoxy click reactions. **K. Jin**, N. Wilmut, W.H. Heath, J. Torkelson*

20:20 – 433. Validity of scaling laws for physical hydrogels. **L. Li***

20:40 – 434. Material design of gel actuator using problem solving techniques by nature. **T. Yamauchi***, T. Nishiyama, T. Hirano, S. Tamesue, T. Mitsumata, K. Hashimoto, N. Tsubokawa, H. Kobayashi

Hawaii Convention Center
Halls I, II, III

Characterization of Polymers and Polymer Assemblies in Solution (#172)

Organized by: T. Sato, T. Yoshizaki,
T. Chang, J. Mays, C. Wu

Poster Session

19:00 – 21:00

435. Dimensional properties of cyclic amylose tris(3,5-dimethylphenylcarbamate) in solution. **A. Ryoki**, H. Ichikawa, S. Kitamura, K. Terao*

436. Dimensional properties of linear and cyclic amylose tris(*n*-octadecylcarbamate) in solution. **A. Ryoki**, S. Kitamura, K. Terao*

437. Conformation and dynamics of polysaccharides and their derivatives in solution. **X. Jiang**, K. Terao, T. INOUE

438. Chain dimensions and intermolecular interactions of polysilanes bearing alkyl side groups over the thermochromism temperature. **X. Jiang**, K. Terao, W. CHUNG, M. NAITO

439. Molecular simulations of helix formation induced by hydrogen-bonding chiral molecules. **K. Horie***, T. Koga

440. Separation of star-shaped polymers with regard to number of arms. **M.I. Malik***, M. Irfan, J. Park, T. Chang

441. Characterization of the chemical composition heterogeneity in poly(styrene-co-butyl acrylate) by RAFT copolymerization. **T. Kawai**, Y. Itoh, K. Sudo, R. Sato

442. HPLC retention behavior of topologically different polymers. **J. Ahn***, Y. Jeong, T. Chang

443. Hysteresis in the phase change of the aqueous solution of the stereo-controlled PNIPAm. **K. Hamamura***, Y. Katsumoto

444. Effect of solvation for the Ludwig-Soret effect of poly(N-isopropylacrylamide) studied in various solvents. **R. Kita***

445. pH-induced reversible control of intramolecular cross-linking of poly(phenylboronic acid). **M. Um**, H. Lee*

446. Facile one-pot preparation of 2D structure based on polymer self-assembly. **S. Shin**, K. Bang, T. Choi*

447. pH-Responsive formation of micelle and vesicle by diblock copolymer in water. **R. Enomoto***, M. Khimani, P. Bahadur, S. Yusa

448. Studies on the formation of polymersomes consisting of photocleavable amphiphilic diblock copolymer and the release of an encapsulated substance. **S. Yamamoto**, J. Nakanishi, S. Nakahama, K. Yamaguchi*

449. Study on relation between spatial distribution and release properties of model drug compounds incorporated in polymeric micelles. **R. Nakanishi**, I. Akiba*, R. Shigeoka

450. pH-responsive polyion complex vesicle. **Y. Tsuda**, K. Nakai, **S. Yusa**, K. Ishihara

451. Size control of polyion complex vesicles covered with phosphobetaine and their uptake of guest molecules. **K. Nakai**, S. Yusa, K. Ishihara

452. Formation of core-shell type micelles composed of polyion complex of cationic block copolymer and anionic polymer. **R. Shigeoka**, I. Akiba*, R. Nakanishi

453. Polyion complex (PIC) micelle composed of pH-responsive anionic unimer micelle and cationic diblock copolymer. **S. Ohno***, S. Yusa, K. Ishihara

454. Self-assembly of binary block copolymer complex driven by intermolecular hydrogen bonding. **S. Nakashima**, I. Akiba*

*** Principle Author**

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455. Adsorption and aggregation properties of homogeneous polyoxypropylene-polyoxyethylene type nonionic surfactants without molecular weight distribution. **S. Yada***, T. Yoshimura

456. Intra- and intermolecular interactions and self-assembly of an amphiphilic alternating copolymer in aqueous solution: complexation with cyclodextrin.

T. Takahashi, T. Sato, K. Terao, A. Hashidzume

457. Adsorption and aggregation properties of hydrocarbon-fluorocarbon hybrid-type gemini surfactants with carboxylates or quaternary ammonium salts.

T. Yoshimura*, A. Morishima, A. Okuda

458. Supramolecular organogel from amphiphilic cyclic peptide self-assembly in organic solvent. **S. Kanazawa**, I. Akiba*, R. Nakanishi

Hawaii Convention Center
Halls I, II, III

Polymers from Renewable Sources and Sustainable Polymer Synthesis (#281)

Organized by: M. Cunningham,
M. Sawamoto, P. Chamapgne,
J. Rawlins

Presiding: M. Cunningham

Poster Session
19:00 – 21:00

459. Sustainable monomers and thermoplastic polymers derived from plant oils via amidation. **L. Yuan**, Z. Wang, N. Trenor, C. Tang*

460. Evaluation of dyeing property using regenerated wool fiber. **R. Yasukawa***, S. Asano, K. Sawada

461. Hydrogels based on Agave tequilana xylans for wound healing. A. Gonzalez, A. Escalante, E. Delgado, J. Gonzalez, P. Gatenholm, **G. Toriz***

462. Hemicelluloses-click-chitosan polymer stabilized palladium (0) as an active catalyst for Suzuki reactions. C. Wu, **M. Song**, X. Peng*, L. Zhong, R. Sun

463. Preparation and characterization of polyurethanes derived from biomass based furan-diols. **S. Shin***, H. Ngo

464. Aliphatic polycarbonates based on carbon dioxide, furfuryl glycidyl ether, and glycidyl methyl ether: Reversible functionalization and crosslinking.

M. Schartenberg, H. Frey

465. Novel surface wrinkling system with natural resources: Morphology control.

N. Okuda, S. Ifuku, M. Morimoto,

H. Saimoto, H. Izawa*

466. Biosynthesis of Poly(3-hydroxyalkanoate) from amino acids in medium with nitrogen, phosphate, and magnesium, or some combination of these nutrients.

T. NAKOIKI*, M. Sakamoto

467. Novel soft materials derived from green-tide-forming chlorophyta.

K. Kanno, S. Takahashi, S. Kato,

Y. Umeno

468. Preparation of high-molecular-weight aliphatic polycarbonates by condensation polymerization of diol and dimethyl carbonate and its various applications.

J. Jeon*, B. Lee*

469. Differences in chemical composition and anatomical structure between juvenile wood and mature wood of cultivated *Larix decidua* Mill. from fast growing tree plantations. **A. Jankowska**,

P. Boruszewski, A. Kurowska, R. Auriga

470. Copolymerization of epoxides with CO₂ catalyzed by multinuclear cobalt complexes. **Y. Hirano**, K. Nakano*

471. Chemical composition of *Populus Hybrida* 275 and *Larix decidua* Mill. wood from fast-growing trees plantations as a new type of raw material for wood-based panels industry. **P.J. Boruszewski***,

A. Jankowska, R. Auriga, M. Maminski,

A. Kurowska, R. Toczyłowska-Marnińska

472. Polymeric sulfur cathodes based on renewable feedstocks. **A. Melker**, C.J. Hawker

473. Novel surface wrinkling system with natural resources: Mechanism.

H. Izawa*, N. Okuda, S. Ifuku,

M. Morimoto, H. Saimoto

474. Ring opening synthesis of polyethylene furanoate (PEF) as a renewable resource based substitute for polyethylene terephthalate (PET). **P. Fleckenstein***, J. Rosenboom*, G. Storti, M. Morbidelli

475. Environment-dependent single-chain mechanics of biomacromolecules and its implications to prebiotic chemical evolution. **S. Cui***

476. Aromatic end-group functionalization as a method to improve mechanical properties of poly(lactic acid). **L. Chile**, A. Wong, P. Mehrkabandavi*, S.G. Hatzikirikos*

477. Cyclic carbonate as building block for sustainable synthesis of non-isocyanate polyurethane elastomers. **G. Beniah**, B.E. Uno, N. Wilmot, W.H. Heath, K. Scheidt, J. Torkelson

478. Tailored adhesion of cellulose substrates by surface modification with block copolymers. **J.L. Engström**, F. Hatton, F. D'Agosto, M. Lansalot, E. Malmstrom, A. Carlmark

479. Novel preparation of hybrid thiol-acrylate/thiol-epoxy materials synthesized using a single base-catalyzed cure.

E. Dhulst, J. Torkelson, W.H. Heath, N. Wilmot

480. Chemical modification on biopolymers for improved functionality in biobased materials. **M.E. Borjesson***

481. Activating polymer production with spinach leaves. **S. Shanmugam***, J. Xu, C. Boyer

482. Preparation of cationic polymerizable imidazolium ionic liquid-acrylamide copolymer and its corrosion inhibition. **Z. Liu***

483. PPC/PPG selectivity dependency on oxidation state of Co/salicy complex.

M. Hatazawa, K. Nozaki

484. Enhanced microwave synthesis of nanostructured polyalanine materials.

M. Gizzadica-Nikolaids*, M. Jevremovic, T. Merian, N. Redon, J. Wojkiewicz, D. Stanisavljev, G. Bowmaker, Z. Zujoyic

485. Living polymerization of renewable methylene butyrolactone monomers using oxidatively activated group transfer polymerization initiators. **Y. Zhang***, E. Chen*

486. Natural polymers reinforced with cellulose nanocrystal to protect the antimicrobial properties of active packaging and beads. **M. Iacriox***

487. Crystalline and functional CO₂-based polycarbonates. **Y. Liu**, W. Ren, X. Lu*

488. Thermal degradation and stability of starch under different processing conditions. **X. Liu**, S. Zhou

Hawaii Convention Center
Halls I, II, III

Sustainable Conversion of Lignin to Value-Added Products and Green Chemicals (#319)

Organized by: X. Zhang, Q. Guo, W. Qin, T. Hu, K. Ramasamy

Presiding: X. Zhang

Poster Session
19:00 – 21:00

489. Synthesize and characterization of 2-pyrone-4,6-dicarboxylic acid derivatives and their charge-transfer complexes. **K. Hiruko***, Y. Kuwana, R. Takahashi, K. Inoue, Y. Otsuka, M. Nakamura, H. Ogata

490. Structure and electronic properties of the charge transfer complexes based on 2-pyrone-4,6-dicarboxylic acid and similar molecules. **R. Takahashi***, Y. Kuwana, K. Hiruko, G.F. Gagabé, Y. Otsuka, M. Nakamura, H. Ogata

491. Structures and physical properties of charge-transfer complexes using a metal-oligoimide intermediate of lignin, 2-pyrone-4,6-dicarboxylic acid. **Y. Kuwana***

492. Lignin model compound bioconversion by versatile peroxidase from *B. adusta*: Mathematical modeling and process control. **N. Busse**, M. Kraume, P. Czermak

493. Influence of lignin on the enzymatic hydrolysis of pretreated biomass substrates. **S. Nakagame***, J.N. Saddler

494. Ti and Au/Ti doped mesoporous materials for the oxidative degradation of lignin.

V. Dufaud*, A. Nunes, L. Djakovitch, D. Da Silva Perez

495. Elucidation of structural features on lignin sub-fractions obtained from sequential solvent fractionation. **S. Park***, J. Kim, H. Hwang, J. Moon, J. Lee, J. Choi

496. Copper on electrospray lignin nanosphere: A catalytic system for azide-alkyne cycloaddition reaction under solvent free condition. **Z. Zhou**, J. Ma, X. Peng*, L. Zhong, R. Sun*

497. Comparative study on topochemistry of hydrothermal delignification from Japanese cedar and Japanese beech.

M. Takada*, E. Minami, H. Kawamoto, S. Saka

Hawaii Convention Center
Halls I, II, III

Polymers for Energy and Optoelectronic Devices (#361)

Organized by: K. Oyaizu, R. Advincula, D. Choi

Poster Session
19:00 – 21:00

498. Liquid crystal photo-alignment characteristics of polyimide with charge transfer complexes. **S. Sato***

499. Transformation process and mechanism between the α -conformation and β -conformation of conjugated polymer Poly(9,9-diethoxyfluorene) in precursor solution. **D. LU**

500. Electrochemical and mechanical properties of polycarbonate/silica nanofiber composite electrolytes. **Z. LI**, H. MATSUMOTO, Y. TOMINAGA

501. Diindeno[1,2-g;1',2'-s]rubicene: All-carbon nonfullerene electron acceptor for efficient bulk-heterojunction polymer solar cells with high open-circuit voltage.

C. Chen*, H. Chen, C. Chen

502. Anisotropic field-effect mobilities of liquid crystalline conjugated polymers on photoaligned insulators. **J. Bae***, S. Han, K. Song

503. Electrochemical characterization of polycarbonate-based electrolytes for all-solid-state Li batteries. **M. Yajima**, Y. TOMINAGA*

504. New water-soluble and crosslinkable binder based on chitosan for Si anode of Li-ion batteries. **M. Cho**, Y. Lee*, C. Chen

505. Broad absorbing and low band gap random copolymers for field effect transistor and polymer solar cell applications.

V. Tamilaran, M. Hyun*

506. Screening for improved bulk heterojunction morphologies of organic semiconductor materials through large-scale Hildebrand solubility parameter calculations. **S.R. Kimura**, D. Yoshidome, H.S. Kwak, M.D. Halls

507. Benzo[1,2-b:4,5-b']dithiophene-functionalized hydrogen-bonding oligothiophene: Self-assembly and photovoltaic properties. **X. Lin**, S. Yagai, T. Kizaki, K. Nakayama

508. Theoretical study of morphology and performance of organic photovoltaics.

E. Kawashima*, M. Fujii, K. Yamashita

509. Electrochemical hydrogenation of poly(4-vinylacetophenone) and its application to a hydrogen storage material.

Y. Shimazaki, R. Kato, K. Oyaizu, K. Nishide*

510. Synthesis and properties of folded π -stacking polymers and their utilization to organic photovoltaic cell.

Y. Naito, C. Matsuno, S. Funyu, S. Okamoto*

511. Optoelectronic properties of polymer composites doped by fullerene derivatives with electron-donating/accepting functionalization.

F. Kim*, H. Song, K. Park, J. Choi, N. Kim

512. Effects of impurity in amorphous conjugated polymer on performance of organic photovoltaics.

J. Kuwabara, N. Takase, T. Yasuda, T. Kanbara

513. High performance ambipolar field-effect transistor based on diketopyrrolopyrrole and benzodithiophene copolymer with cyanovinylene linkage.

J. Park, S. Park, S. Park, S. Park*

514. Synthesis and characterizations of polyamides and polyimides containing indolo[3,2-b]carbazole moiety in main-chain or side-chain.

R. Ueno, T. Yoshihi, T. Mimura, Y. Nagase*, M. Kawamoto

515. Flexible organic photovoltaics on polyethylene terephthalate substrate prepared by low-temperature process.

T. Kuwabara*, W. Xiaofan, T. Yamaguchi, T. Taima, K. Takahashi

516. Synthesis and properties of bisphenol B novolac resin as a photo-resist material.

T. Nishimura, H. Yamasaki*

517. New electrochromic polymers based on Tröger's base.

W. Li, T. Michinobu

518. Helix-sense-selective polymerization of 3,5-bis(hydroxymethyl)phenylacetylene bearing rigid and branched aryl groups and their chiroptical properties.

Z. Shi, M. Teraguchi, T. Aoki, T. Kaneko

519. Simplified electrochemical polymerization to fabricate a PEDOT hole injection/transport layer.

T. Matsushima*, S. Katori, K. Hiroki

520. Synthesis and characterization of poly(arylenevinylene)s by ring-opening metathesis polymerization.

C. Yu*, S. Wen, C. Wang

521. Electrocatalytic hydrogenation of pyridine polymers and their application to a hydrogen storage material.

T. Ooya, R. Kato, K. Oyaizu, H. Nishide*

522. Nitrogen atom substitution in benzodiazole of conjugated polymer for high performance polymer solar cells.

E. Jung, J. Jung, J. Jo, W. Jo

523. Conjugated random copolymers consisting of pyridine- and thiophene-capped diketopyrrolopyrrole as co-electron accepting unit for efficient polymer solar cells.

J. Lee, W. Jo

524. Photovoltaic behavior of inverted polymer solar cells using indium tin oxide electrodes modified by piperazine derivatives.

T. Kusumi, K. Fujimori, T. Kuwabara, T. Yamaguchi, T. Taima, K. Takahashi*

525. Synthesis and characterizations of pendant type poly(acryl amide) containing indolo[3,2-b]carbazole moiety.

T. Mimura, M. Kawamoto, Y. Nagase*

526. Spectroscopic ellipsometry and FTIR-ATR study on removal stage of solvent in spin-coated PEDOT:PSS on crystalline-Si. H. Shirai*, S. Funada, Q. Liu, R. Ishikawa, K. Ueno

527. Chemical mist deposition of organic and inorganic films on textured c-Si for efficient crystalline-Si/organic heterojunction solar cells. H. Shirai, T. Ohki, K. Ichikawa, H. Jaker, R. Ichikawa, K. Ueno

528. Insight into the energy loss in organic solar cells based on benzothiophene copolymers.

E. Al-Naamani, M. Ide, A. Gopal, A. Saeki*, I. Osaka, S. Seki

529. Carbazole-assisted electrodeposition of graphene oxide.

P. Advincula*, J. Mangadlao, R. Advincula*

530. Spectroscopic studies of curing and alignment mechanisms of photoreactive mesogen molecules.

K. Song*, J. Jung

531. Molecular engineering of benzothieno-oisoindigo copolymers allowing highly preferential face-on orientations.

M. Ide*

* Principle Author

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<http://pacificchem.org/onlineprogram>

- 532.** Low bandgap polymer nanofiber-based organic photovoltaic devices processed in ambient air. **T. Kim**, S. Yang, **C. Park**
- 533.** Syntheses of benzene type step- π -conjugated polymer and study on photoinduced electron transfer. **H. Guo***, H. Aota
- 534.** Development of new hole-transporting polypeptid materials and their charge-transport properties. **S. Itazawa**, K. Karino, M. Ichikawa, T. Uchida, T. Hiejima*
- 535.** Syntheses of benzene type step- π -conjugated polymer and study on photoinduced energy transfer. **Y. Ishikawa***, H. Aota
- 536.** Step- π -conjugated polymer as macro-molecular wire. **H. Aota***
- 537.** On the anomalous temperature dependence of intrinsic birefringence for polymers. **Y. Okada**, O. Urakawa, T. INOUE*
- 538.** Synthesis and electrochemical properties of radical polymer containing anionic group for a high energy density organic secondary battery. **T. Murata**, H. Tokue, K. Oyaizu, H. Nishide*
- 539.** Charge-discharge performance of TEMPO-containing polymer particles under flow conditions. **R. Watanabe**, R. Sakazaki, H. Tokue, K. Oyaizu, H. Nishide
- 540.** Development of protic ionic liquid-based polymer electrolytes with toughness for polymer electrolyte fuel cells. **S. Honma**, T. Morinaga, R. Shomura, T. Sato, T. Mori, K. Ohno, Y. Tsuji
- 541.** Simultaneous enhancement of upconversion and downshifting luminescence via plasmonic structure. **J. Park**, D. Ko
- 542.** Solid state NMR studies on the aggregated structures and properties of polymer:fullerene bulk heterojunction films with solvent additives. **S. Kawano**, H. Ogata
- 543.** Fiber-based flexible electrode for electrochemical supercapacitor with high capacitance. **J. Lee***

Thursday Morning

Hawaii Convention Center
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NMR Spectroscopy of Polymers and Biobased Materials (#12)

- Organized by:* H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madson, K. Saalwachter, Y. Yao, J. Battiste
Presiding: A. English, J.L. White
- 8:00 – 544.** NMR measurement of relative chain orientations over >10 nm and of chain end location in polyethylenes: Structural models without excess density. **K. Schmidt-Rohr**, K.J. Fritzsching, K. Mao, A.W. Bosse
- 8:25 – 545.** Solid state NMR guides the design of tailored physical properties in gradient copolymers. **J.L. White**, J. Sigle, A. Clough
- 8:50 – 546.** Interchain proximity of polystyrene explored by solid-state NMR. **X. Wang***, P. Sun, Q. Xue
- 9:15 – 547.** Solid-state ^{33}S NMR of polymers. **K. Yamada***
- 9:40** Break
- 9:55 – 548.** Organic light-emitting diodes and organic solar cells: NMR analysis toward higher performance. **H. Kaji***, T. Fukushima, K. Suzuki, K. Shizu
- 10:20 – 549.** Direct measurements of donor/acceptor interfaces in organic photovoltaics via heteronuclear recoupling experiments. **R. Nieuwendaal**, D. Delongchamp, A. Sieval, J. Hummelen, M. Heeney, Z. Fei
- 10:45 – 550.** Accessing molecular motion features in polymers using dipolar filtered time domain NMR signals at low field. U.B. da Silva, M.F. Cobo, m.N. DEURÍDICE, E.R. deAzevedo*
- 11:10 – 551.** Relayed dynamic nuclear polarization to probe micro structures. A. Pinon, P. Berruyer, J. Schlaginweit, A. Rossini, A. Lesage, **L. Emsley**

Hawaii Convention Center
325B

New Perspectives of Synthetic and Biological Soft Matter (#57)

- Organized by:* F. Horkay, J. Douglas, N. Choudhury, H. Jinnai
Presiding: J.F. Douglas, G. Wnek
- 8:00** Opening remarks
- 8:05 – 552.** Fast and complete thixotropic recovery of molecular organogels. **R.G. Weiss**, V. Mallia
- 8:35 – 553.** Soft functional materials from bile salts. S. Chatterjee, T. Gorai, M. Maiti, **U. Maitra***
- 9:05 – 554.** Biomimetic tough hydrogels for biomedical applications. **N. Roy Choudhury***, J. Whittaker, N.K. Dutta, C.M. Elvin, A.J. Hill
- 9:35** Break
- 9:50 – 555.** Self-assembly and interactions in biopolymer systems. **F. Horkay***, P. Baser
- 10:20 – 556.** Amphiphilic hyperbranched dendritic-linear polymers for drug-delivery applications. **E. Malmstrom***, C. Porsch, A. Nyström, Y. Zhang
- 10:50 – 557.** Spatially controlled surface modification of coextruded PCL nanofibers as cell responsive biomaterials. **S. Kim**, J. Pokorski*
- 11:10 – 558.** Two stem microfluidic generation of aqueous alginate multicompartment capsules and their application in bacterial quorum sensing. A. Lu, **S.R. Raghavan**, J. Terrell, W. Bentley
- Hawaii Convention Center
Halls I, II, III

Polymer Gels as Advanced Soft Materials (#83)

- Organized by:* R. Yoshida, T. Miyata, F. Winnik, J. Aizenberg
- Poster Session**
10:00 – 12:00
- 559.** Stimuli responsive and self-healing supramolecular materials through host and guest interactions. **Y. Takashima**, A. Harada
- 560.** Self-healing materials based on polyrotaxane-boronate interactions. **S. Mori**, M. Nakahata, Y. Takashima, A. Harada*
- 561.** Functional supramolecular polymeric materials based on redox-responsive host-guest interaction. **M. Nakahata**, Y. Takashima, A. Harada*
- 562.** Macroscopic artificial muscle powered by the microscopic sliding motion of [2]daisy chain. **K. Iwaso***, Y. Takashima, A. Harada*
- 563.** Supramolecular gelation of functional liquids and their dielectric properties. **R. YAMAMOTO**, Y. MINAMI, J.K. Hui, M. Morikawa, N. Kimizuka*
- 564.** Rotaxane cross-linked polymers synthesized with macromolecular [2]rotaxane cross-linker. **J. Sawada***, D. Aoki, T. Takata
- 565.** Effects of both amines and acid in supramolecular hydrogel formation of contained tetracarboxylic acids calix[4]arene gelator. **H. Choi***, J. Lee, J. Jung*
- 566.** Pyridine-based supramolecular gel induced by hydrazone bond and its properties. **Y. Choi**, J. Jung*, J. Lee, S. Jung
- 567.** Supramolecular gels with high strength by tuning of calix[4]arene-derived networks. **J. Lee**, J. Jung*
- 568.** Relationship between mesoscopic heterogeneity and re-gelation behavior of a supramolecular network. **Y. Matsumoto**, A. Shundo, K. Matsumoto, M. Ohno, N. Tsuruzoe, M. Goto, K. Tanaka*
- 569.** Evaluation of fracture behavior for polymer gels with controlled network structure. **Y. Akagi***, T. Sakai
- 570.** Design of hydrogels with controlled swelling properties by tuning the chemical structure of polymer backbones. **H. Kamata***, U. Chung, T. Sakai

571. Hydrogel with a reliable deformation region in an aqueous environment. **S. Kondo**, T. Hiroi, U. Chung, M. Shibayama, T. Sakai

- 572.** Electrophoretic mobility of double stranded DNA in defect controlled polymer networks: Relation to correlation length and mesh size. **K. Kharulina**, X. Li, K. Nishi, M. Shibayama, U. Chung, T. Sakai
- 573.** High-toughness ion gel with controlled polymer network. **K. Hashimoto***, K. Fujii, T. Sakai, M. Shibayama
- 574.** Analysis of electrostatic interaction causing high sliding friction of polyzwitte-rionic hydrogel. J. Ahmed, **T. KUROKAWA**, H. Guo, T. Yamamoto, M. Takahata, T. Nakajima, J. Gong*
- 575.** Novel double-network hydrogel directly bondable to the bone and its application to fixation of artificial cartilage and ligament. **T. Nonoyama**, S. Wada, R. Kiyma, N. Kitamura, M. Mredha, X. Zhang, T. KUROKAWA, T. Nakajima, Y. Takagi, K. Yasuda, J. Gong*

- 576.** Controlling superstructure of rigid polyelectrolytes in oppositely charged hydrogels via programmed internal stress.

- 577.** Stiffness of hydrogels: Novel hydrogel immobilization method on bone tissue. **R. Kiyma**, T. Nonoyama, S. Wada, N. Kitamura, T. KUROKAWA, T. Nakajima, K. Yasuda, J. Gong*

- 578.** Stimuli-responsive gel consisted of rigid inorganic nanotube "imogolite". **K. Shikinaka***, K. Kaneda, T. Maki, H. Masunaga, Y. Osada, K. Shigehara

- 579.** Synthesis and mechanical properties of joint-linker gels with reversible redox sol-gel transition. **K. Moriyama***, N. Naga, K. Takase, H. Furukawa

- 580.** Extremely tough and elastic hydrogel using macro-crosslinkers. **S.K. Goswami***, J. McAdam, L. Hanton, S. Moratti

- 581.** Shutdown of ionic conductivity for an ion gel functionalized by LCST thermosensitive polymer. **Y. Kobayashi***, Y. Kitazawa, H. Kokubo, M. Watanabe

- 582.** Study of ionic liquid-polymer dielectric layer for high-performance flexible thin film transistors. **J. Ko**, K. Lim, C. Jo, N. Cho, J. Park, Y. Kim, Y. Kim*

- 583.** Radiation-induced syntheses and applications of novel polymeric ionic liquid gels. **M. Zhai**, S. Wang, X. Zhang, J. Peng
- 584.** Rational design of ionic-liquid-gel surfaces with easy-sliding and ultra-durable features. **H. Liu***, L. Jiang

- 585.** Small-angle X-ray scattering studied on thermoresponsive microgels. **T. Kureha**, S. Matsui, T. Shibamoto, T. Watanabe, T. Sato, D. Suzuki*

- 586.** Synthesis and structural evaluation of microgels integrated by the star polymers in the submicron-sized water droplets. **T. Shibamoto**, T. Kureha, S. Matsui, T. Sakai, D. Suzuki*

- 587.** Preparation and properties of moisture-absorbing film impregnated with sodium polyacrylate and polyurethane. **J. Lee**, D. Jeong, S. Ko, S. Park, S. Hwang, S. Lee*

- 588.** Preparation of glucose-responsive shape-memory hydrogels using molecular complexes as dynamic crosslinks. **M. Hayashi**, A. Kawamura, T. Miyata*

- 589.** Synthesis of responsive hydrogels with protein recognition sites by molecular imprinting and their recognition behaviors. **Y. Masui**, A. Kawamura, T. Miyata*

- 590.** Synthesis of dual stimuli-responsive polymers that undergo sol-gel phase transition by light and biomolecule. **K. Okuma**, A. Kawamura, T. Miyata*

- 591.** Formation of dynamic biomolecular recognition sites in smart hydrogels by molecular imprinting and their recognition control. **Y. Kuriu**, A. Kawamura, T. Miyata*

- 592.** Network structure and responsive behavior of temperature-responsive hydrogels synthesized by controlled radical polymerization. **C. Norioka**, A. Kawamura, T. Miyata

- 593.** Preparation of prostaglandin-imprinted hydrogels with cyclodextrin and their responsive behavior. **Y. Tanaka**, A. Kawamura, T. Miyata*

- 594.** Relationship between gel network and molecular recognition of stimuli-responsive hydrogels with cyclodextrins. **S. Yamafuji**, A. Kawamura, T. Miyata*

- 595.** Modular and injectable poly(oligoethylene glycol methacrylate)-based hydrogels with tunable physicochemical and biological interactions. **E. Bakai***, N.M. Smeets, T. Hoare

- 596.** Metal ion-responsive biodegradable hydrogels made of PEG-DNA copolymers. **S. Tanaka**, K. Fukushima, K. Wakabayashi, A. Kuzuya*, Y. Ohya

- 597.** New robust biodegradable platform for the engineering of macromolecules for consumer and biomedical applications. **H. Ye***

- 598.** 3D perfusion culture through patterned photodegradable hydrogels. **F. Yanagawa***, M. Tamura, S. Suguri, T. Takagi, K. Sumaru, T. Kanamori

- 599.** Investigation of new cooling systems based on copolymers of temperature-responsive poly(N-isopropylacrylamide) with butyl acrylate and vinyl acetate. **H. Sasaki**, H. Honda, Y. Kita, K. Sekimoto, H. Tsukada, A. Tosaka, A. Sasaki, M. Kadokura

- 600.** Thermoresponsive strong anionic copolymer brushes grafted silica beads for effective cation exchange chromatography. **K. Nagase***, J. Kobayashi, A. Kikuchi, Y. Akiyama, H. Kanazawa, T. Okano

- 601.** Self-oscillating polymer brushes: Design of autonomous functional surfaces exhibiting spatio-temporal property changes. **T. Masuda**, K. Homma, A. Mizutani Akimoto, K. Nagase, T. Okano, R. Yoshida

- 602.** Self-oscillating multiblock copolymers with dynamic viscoelastic oscillation. **M. Onoda***, T. Ueki, M. Shibayama, R. Yoshida

- 603.** Biphasic electroactive hydrogel: Integrating microelectronics and biotechnology. **z. shi***, G. Yang

- 604.** Controlled drug release of core (poly-N-isopropylacrylamide- β -cyclodextrine) shell (poly-N-isopropylacrylamide) gels. J. Gutierrez, E. Delgado, **G. Toriz**, M. Rabelero

- 605.** Nanogel tectonics materials: Preparation and characterization of nanogel-crosslinked hybrid film. **S. Mukai**, Y. Hashimoto, Y. Tahara, S. Sawada, K. Akiyoshi

- 606.** Protein-mimic strategies to design hydrogel particles that reversibly captures target ions. **Y. Hoshino***, M. Yue, T. Miyoshi, Y. Miura

- 607.** HPG/PVC thermoresponsive nanogels for drug delivery. **J. Bergueiro***, S. Wedepohl, M. Calderon

- 608.** Self-assembly of brush block copolymers to nanostructured materials. **A. Chang**, R.H. Grubbs

- 609.** One-pot synthesis of poly(N-isopropylacrylamide) gels with nearly-ideal polymer network structure. **Y. Jochi***, Y. Takeoka, T. Seki, K. Satoh, M. Kamigaito

* Principle Author

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- 610.** Effect of composition ratio on electrical conductivity of PEDOT/PSS nanogels. **T. Horii***, H. Hikawa, M. Katsunuma, Y. Li, H. Okuzaki
- 611.** PEDOT/PSS/Polyglycerin composite for stretchable electrodes. **M. Sato**, R. Tanigawa, T. Kubota, H. Okuzaki
- 612.** All-organic supercapacitors using PEDOT/PSS as flexible electrodes. **H. Takezawa***, M. Katsunuma, M. Sato, H. Okuzaki
- 613.** Synthesis and characterization of PEDOT/PSS with conductivities higher than 1000 S/cm. **H. Amemiya**, T. Horii, H. Okuzaki
- 614.** Stretchable and highly conductive polymer gels. **T. Kubota**, K. Iwashita, H. Okuzaki
- 615.** Ammonium oxidation reaction catalyzed by bacteria entrapped within macroporous polymeric hydrogels using a suspension-gelation method. **R. Sato***, R. Noma, H. Tokuyama
- 616.** Temperature-swing adsorption of metal ions onto thiol-functionalized thermosensitive gels. **M. Onodera***, H. Tokuyama
- 617.** Esterification in organic media using lipase immobilized within amphiphilic NIPA-co-PEGMEA gels. **H. Tokuyama***, R. Sato, A. Sato
- 618.** Preparation of anisotropic physical hydrogels of cyanobacterial polysaccharides. **M. Okajima**, R. Mishima, T. Kaneko*
- 619.** Orientation mechanism of rigid polysaccharides on gas-liquid/solid-liquid interfaces and application to anisotropic materials. **K. Okeyoshi**, M. Okajima, T. Kaneko
- 620.** 1D swelling of in-plane oriented hydrogels of supergiant LC polysaccharides. **K. Amornwachirabodee***, M. Okajima, T. Kaneko
- 621.** Effect of side chain structure on helix-helix transition of polypeptide hybrid gels. **Y. Mizuno***, H. Furuya
- 622.** Physical hydrogels based on multifunctional polyurethanes via ionic or acidic crosslinking. **M. Nguyen-Kim***, J.C. Licht, J.C. Borghs, A. Böker
- 623.** SAXS and SANS study on phase-separated structure of amphiphilic gel composed of poly(dimethylsiloxane) and poly(*N,N*-dimethyl acrylamide) in solvated state. **K. Yamamoto***, Y. Mori, E. Ito
- 624.** Time-resolved SANS study to determine the chain exchange kinetics of associative network micelles. **D.G. Abebe**, K. Liu, S. Mishra, A. Wu, T. Fujiwara*
- 625.** Molecularly imprinted polymers prepared using posteriori cross-linking methodology of functional polymer species. **K. Yoshikawa***, Y. Kitayama, T. Takeuchi
- 626.** Molecular simulation of structure and mechanical properties of gels formed by end-linking of tetra-arm polymers. **H. Tanaka***, H. Ozaki, T. Koga
- 627.** Stimuli-responsiveness of hydrogels originated from the supramolecular interactions depending on polymer network structure. **S. Noguchi**, S. Tamesue*, Y. Kimura, T. Mitsumata, N. Tsubokawa, T. Yamuchi
- 628.** Effect of solution composition on the thermoresponsive CO₂ adsorption/desorption properties of poly(N-isopropylacrylamide)-polyamine copolymer gel. **Y. Amano**, Y. Seida*, E. Furuya
- 629.** Synthesis and property of nano-templated functioned gel. **T. Miyamae***
- 630.** Photostimulated swelling behaviors of polypeptide gel containing azobenzene units. **T. Aso**, T. Okamura, T. Hiejima
- 631.** Photostimulation induced expansion-contraction of uniaxially oriented liquid crystalline polypeptide gel containing spiropyran units. **H. Imai**, A. Akai, T. Hiejima*

Hawaii Convention Center
Halls I, II, III

Controlled Macromolecular and Supramolecular Architectures for Sustainability (#112)

Organized by: M. Kamigaito, C. Hawker, G. Qiao, K. Wooley, E. Yashima

Poster Session

10:00 – 12:00

- 632.** Acrylonitrile-conjugated diene copolymers by Ru-catalyzed living radical copolymerization. **F. Bando**, M. Uchi, M. Sawamoto
- 633.** Reversible addition-fragmentation chain transfer polymerization of hydroxy-functional vinyl ethers. **S. Sugihara***, Y. Maeda, Y. Kawamoto
- 634.** Design of electrophoretic acrylic polymer synthesized via atom transfer radical polymerization. **T. Kameyama**, A. Takasus
- 635.** Photo-induced switchable living cationic and radical polymerization. **R. Ishibashi**, K. Satoh, M. Kamigaito*
- 636.** Polymerization mediated by RAFT agents bearing cyclodextrin moieties. **K. Koyanagi**, Y. Takashima, A. Harada
- 637.** Highly recyclable imidazolium-function-al β-cyclodextrin catalyst for the Heck coupling reaction in water. **S. Fortun**, A.R. Schmitz*
- 638.** Living cationic polymerization via degenerative chain transfer on C–S bond. **M. Uchiyama**, K. Satoh, M. Kamigaito*
- 639.** Halogenation of growing anionic species in living anionic polymerization of hydrocarbon monomers for subsequent mechanistic transformation. **Y. Mori**, K. Satoh, M. Kamigaito*
- 640.** Silylum-catalyzed living methacrylate polymerization via *in situ* hydrosilylation of monomer. **T. Xu**
- 641.** Investigation of Ni-catalyzed catalyst-transfer Suzuki-Miyaura cross-coupling polymerization for the synthesis of polyphenylene. **K. Kosaka**, K. SUZUKI, H. OKAMOTO, Y. Ohta, T. Yokozawa
- 642.** Palladium catalyzed chain-growth polycondensation of fluorene by direct lithium-halogen cross-coupling reactions. **Y. Qiu**, K. Noonan
- 643.** Model reactions for catalyst-transfer condensation polymerization of symmetric donor-acceptor-donor and acceptor-donor-acceptor triaryl monomers. **Y. Tokita**, T. Yokozawa*, Y. Ohta, m. Katoh
- 644.** Highly active and syndioselective zinc complexes for the ring-opening polymerization of β-Butyrolactone. **T. Ebrahimi**, S.G. Hatzikiriakos, P. Mehrkhodavandi*
- 645.** Control of molecular weight and end-functional groups of polyesters by means of A₂ + B₂ polycondensation and cross metathesis. **R. Okabayashi**, Y. Ohta, T. Yokozawa*
- 646.** Proton-transfer polymerization (HTP); Converting commercially available and biomass-derived dimethacrylates into polyesters by *N*-heterocyclic carbenes. **M. Hong**, E. Chen*
- 647.** Enzymatic synthesis and characterization of cellulose-based composite hydrogels. **Y. Hata**, T. Sawada, T. Serizawa*
- 648.** Dynamic hybridization mechanisms of glucans with water-soluble polythiophene. **G. Fukuhara**, M. Imai, D. Fuentelba, K. Tamano, M. Sasaki, C. Yang, T. Mori, U. Hiroshi, C. Bohne, Y. Inoue
- 649.** Synthesis of polypeptides by means of chain-growth condensation polymerization of amino acid monomers bonded to polynorbornene copolymers. **A. Morimitsu**, Y. Ohta, T. Yokozawa
- 650.** Proton conduction in a cephalopod structural protein. **D.D. Ordinario***, L. Phan, W.G. Walkup IV, J. Jocsón, E. Karshalev, N. Husken, A.A. Gorodetsky
- 651.** Synthesis and conformational analysis of a double-stranded helical foldamer. **T. Tsuda**, N. Ousaka, E. Yashima*

- 652.** Synthesis of novel multistaranded copolymers by postpolymerization of template Poly(substituted phenylacetylenes). **K. Sono**, K. Matsui, Y. Zang, T. Aoki, M. Teraguchi, T. Kaneko
- 653.** Synthesis and association behavior of a carboxylic acid tetramer connected through chiral amide and o-phenylene diethynylene linkers. **Y. Nakajima**, J. Tanabe, N. Ousaka, E. Yashima

- 654.** Helix-sense-selective photodegradation of racemic helical Poly(substituted phenylacetylene)s by highly selective photocyclic aromatization (SCAT) using circularly polarized light (CPL). **M. Miyata**, M. Teraguchi, T. Kaneko, T. Aoki
- 655.** Synthesis of helical poly(phenylacetylene)s bearing chiral and achiral imidazolidinone pendants and their application to asymmetric organocatalysis. **K. Shimomura**, T. Leandro, H. Iida, K. Hayashi, A. Dos Santos, E. Yashima*

- 656.** In-chain ring polyacrylamides via molecular-recognition-assisted living radical cyclopolymerization: Precision synthesis and novel properties. **Y. Kimura**, T. Terashima*, M. Sawamoto*

- 657.** Synthesis and property of mechanically linked block copolymers derived from functional macromolecular [2]rotaxanes. **D. Aoki***, S. Uchida, T. Takata
- 658.** Controlled assembly of π-conjugated molecules with multiple stimuli. **V.R. Kotagiri**, D. Miyajima, T. Aida*

- 659.** Synthesis of main- and side-chain sequenced polymers via radical (Co)polymerization of maleimide-function- alized sequence-regulated oligomonomers. **T. Soejima**, K. Satoh*, M. Kamigaito*
- 660.** Synthesis of a brush macromolecule composed of a poly(acrylate ester) main chain and carbon-dioxide-derived poly(propylene carbonate) side chains. **S. Honda**, H. Sugimoto

- 661.** Synthesis-like self-assembly of tooth-brush-like block copolymers with water-soluble comb-block and thermoresponsive PNIPAM block. **H. Kubosawa**, D. Yao, R. Jin*
- 662.** Crosslinked single-chain block copolymers via living radical polymerization: Connected microgel spheres. **M. Matsumoto**, T. Terashima*, M. Sawamoto*

- 663.** Synthesis and microphase separation of well-defined hyperbranched poly- amide-*b*-poly(methyl methacrylate). **K. Sakurai**, K. Hosoya, Y. Ohta, T. Yokozawa*
- 664.** Imine-based microgel star polymers: Precision network π-conjugated nanospace. **Y. Azuma**, T. Terashima*, M. Sawamoto*

- 665.** In situ nanoparticulation of fully conjugated block copolymers containing polythiophene. **I. LEE**
- 666.** Synthesis and characterization of amphiphilic diblock copolymer using photodegradable heterobifunctional crosslinking reagent bearing alkyne protected by silyl group and maleimide. **S. Yamazaki**, S. Yamamoto, S. Nakahama, K. Yamaguchi

- 667.** Renaissance of a forgotten polymer: Branched polybis(chloromethyl)oxetane. **E. Christ***, H. Frey
- 668.** Novel synthetic method of polymer nitrile *N*-oxide and application to catalyst-free polymer linking. **T. Tsutsuba**, H. Sogawa, T. Takata

- 669.** Structurally-dynamic hydrogels based on 1,2-dithiolanes. **X. Zhang***, R. Waymouth*
- 670.** Synthesis of linear poly(ethyleneimine-*b*-hyperbranched polyamide and transcription of its self-assembled structures to silica by silification. **Y. Ohta**, K. Sakamoto, D. Inoue, M. Saito, R. Jin, T. Yokozawa*
- 671.** Precise synthesis of organic/inorganic hybrid polyamide and characterization of its nano structure. **Y. Nagae***, T. Ohishi, M. Kido, M. Sato, K. Kojo, T. Hirai, A. Takahara

- 672.** Synthesis of self-standing 2D polymer membranes (7): By ADMET 2D polymerization of supramolecular polymers of cyclic trimers of phenylacetylenes prepared by highly selective photocyclic aromatization. **S. Sato**, T. Aoki, M. Teraguchi, T. Kaneko
- 673.** Preparation of functional properties in well-controlled stereoregular polymer brushes using living anionic polymerization method. **M. Sato***, Y. Higaki, N. Ohta, K. Kojo, T. Hirai, A. Takahara

- 674.** Molar mass change of a modified polyamide and its effect on the melt flow behavior. **Y.P. Seo**, **Y. Seo***

Hawaii Convention Center
326A

Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158)

Organized by: T. Meyer, M. Uchi, H. Sleiman, Z. Li
Presiding: T.Y. Meyer

8:00 Welcoming Remarks

- 8:05 – 675.** Controlling structure in functionalized polymers prepared using metathesis. **M. Hillmyer***

- 8:35 – 676.** Synthesis of functional polymers using controlled polymerization. **R.H. Grubbs***

- 9:05 – 677.** Preparation of sequenced copolymers using entropy-driven ring-opening polymerization. **R.M. Weiss**, A.L. Short, T.Y. Meyer*

- 9:35 – 678.** New precision structures of polyethylene. **K.B. Wagener***, A.S. Veige, H. Li

10:05 Break

- 10:15 – 679.** Sequence-controlled polymers: About monomer-coded information, structure, and function. **J. Lutz***

- 10:45 – 680.** General approach to sequence-controlled polymers through macrocyclic ROMP. **W.R. Gutekunst***, C.J. Hawker

- 11:15 – 681.** Tapered block copolymers: Controlling segment sequence to improve materials properties. **T. Epps***, W. Kuan

Hawaii Convention Center
323C

Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194)

Organized by: K. Tanaka, A. Crosby, S. Kim, K. Dalnoki-Veress
Presiding: A.J. Crosby, H. Yabu

- 8:00 – 682.** Controlling crystallization of, and with, conjugated polymers at interfaces. **R. Hayward**

- 8:30 – 683.** New approach to dissolved air flotation: Bubble surface modification using tailored polymers. **A.M. Granville***, R.K. Henderson*, N. Hanumanth Rao, R. Yap

- 8:45 – 684.** Distribution of glass transition temperature in polymer thin films by neutron reflectivity and low energy muon spin relaxation. **T. Kanaya**, H. Ogawa, R. Inoue, T. Prokscha

- 9:00 – 685.** Structure and adhesion of crystalline polymer interfaces. **T. NISHINO***

- 9:30 – 686.** Surface mediated self-assembly of biopolymers. **Z. Fakhraai***

* Principle Author

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10:00 – 687. On-demand liquid transportation using bioinspired omniphobic lubricated surfaces based on honeycomb and pincushion films prepared by self-organization. J. Kamei*, H. Yabu

10:15 – 688. Lamellar structure formation in poly(*N*-dodecylacrylamide) by humidity annealing. J. Matsui*, Y. Hashimoto, T. Sato, S. Nagano, Y. Nagao, M. Mitsubishi

10:30 – 689. Phase behavior of diblock copolymers in spherical 3D confinement. T. Higuchi*, M. Pinna, A.V. Zvelindovsky, H. Jinmai, H. Yabu

10:45 – 690. New design of block copolymers for sub-10 nm features and perpendicular orientation by thermal annealing. T. Seshimo, D. Kawana, K. Ohmori, T. Hayakawa

11:00 – 691. Probing molecular structures of buried polymer interfaces in situ. Z. Chen*

11:15 – 692. Plastic deformation mechanisms in semicrystalline and nanostructured block copolymers. J. Rottler, S. Jabbari-Farouji, A. Parker, O. Lame, A. Makke, M. Perez, J. Barrat

Hawaii Convention Center
Halls I, II, III

Functional Materials Based on Organic-inorganic Hybrid Polymers (#221)

Organized by: K. Naka, F. Jaekle, C. Ha, J. Ohshita

Presiding: F. Jaekle, K. Naka, J. Ohshita

Poster Session

10:00 – 12:00

693. Triple stimuli-responsive ferrocene-containing PEG-based materials for surface-modification and nanocapsules. A. Alkan*, F.R. Wurm

694. Fabrication of hydrophilic electrospun fiber blends. S. Ali*, S. Kim

695. Self-assembly of metal organic materials incorporating 1,3-adamantanedicarboxylic acid and 1,3 bis(4-pyridyl) propane for tuning of polymer properties. C.V. Gauthier*, J.P. Harmon, J.J. Flanagan, G. Beggs, G. Craft, A. Lopez

696. Synthesis and properties of boron/silicon bimetallic copolymers. P. Puneet, R. Vedarajan, N. Matsumi

697. Synthesis of redox-responsive polymer nanostructures containing ferrocene moieties by living coordination polymerization of allene derivatives. H. Eguchi, H. Nishiyama, S. Inagi, I. Tomita

698. Fabrication of functionally advantageous highly filled nanocomposites by employing new reactor granule technology. B. Mairia*, M. Terano, T. Toshiaki

699. Thermal diffusion of carbon molecule into polytetrafluoroethylene. M. Ito*

700. Investigation of the crosslinking mechanism of multifunctionalized POSS/PU composites by rheology. Q. Zhang*, K. Xi, X. Jia*

701. Sacrificial reducing agent free photoinduced green synthesis of metal nanoparticles over polythiophene foam/TiO₂ nanocomposite. R. Badam*, R. Vedarajan, N. Matsumi

702. In situ formation of honeycomb silicon-containing polymer-derived ceramics by a hybrid strategy involving plasma and pyrolysis. J. Gong*, B. Xu, X. Tao

703. Structure and physical properties of chiral [MnCr(oxalate)₃] crystals with supramolecular cations. M. Yoshitake*, K. Kubo, S. Nishihara, K. Inoue, T. Akutagawa, S. Noro, T. Nakamura

704. Synthesis of element-block polymers from para-disubstituted T8-caged silsesquioxane monomers. T. Maegawa*, Y. Irie, H. Imoto, K. Naka*

705. Properties of polyimides from bis(3-aminopropyl) hexaisobutyl substituted T8-caged silsesquioxane. O. Miyashita*, T. Maegawa, Y. Irie, H. Imoto, K. Naka*

706. Controlled polymerization of vinyl monomers by visible light-induced Si-ATRP on titania/reduced graphene oxide nanocomposite. A. Bansal*, A. Kumar, S. Jain, S. Ray

707. Transparent and high-dielectric polymer composite film consisting of densely polymer-grafted inorganic particles. N. Iwata, O. Sato, K. Ohno, M. Tokita*

708. Coating of inorganic particles or fibers with conducting polyanilines and their electrical conduction and corrosion protection properties. S. Lee*

709. Synthesis and properties of polybenzoxazine-silica nanocomposites provided from perhydropolysilazane. J. Lee*, R. Saito*

710. Development of shuttle adsorbent between the bottom and surface of water for adsorption of pollutants. Y. Miura*, S. Itoh, S. Tanaka

711. Chiral crystals of inorganic-organic hybrids based on polyoxometalates and supramolecular cations. J. Xiong*, K. Kubo, S. Noro, T. Nakamura*

712. Preparation and gas barrier properties of silica/chitosan organic-inorganic hybrid gas barrier membranes via sol-gel method. K. Kuraoka, R. Yamamoto

713. Electric heating films based on biopolyurethane nanocomposites containing carbon nanotube. B.G. Min*, S.G. Kang

714. Luminescent dendrimers using typical elements. T. Kambe*, T. Imaoka, K. Yamamoto

715. Fabrication of flower-like nickel oxide hollow spheres with enhanced supercapacitive performance. L. Huang*

716. Hybrid polyphosphazene containing two symmetrical polyhedral oligomeric silsesquioxane (POSS) units. I. HWANG, J. LIM, K. Kim*

717. One-pot synthesis of gold-polymer hybrid nanoparticles and tuning of their structures and colors. Y. Fukui*, K. Fujimoto*

718. Self-assembled carbon nanotube-incorporated polymer films using mixed metal-terpyridine complexes: Enhancement of photoinduced electron transfer. D. Jeong, Y. Lee, C. Song*

719. Preparation of organic solvent-dispersible titanium oxide/silsesquioxane hybrid nanoparticle. K. Imai

720. Synthesis of D-A polymers with dilanobiphenole donor and pyridine or pyrazine acceptor and their applications to dye-sensitized solar cells. Y. Adachi, J. Ohshita*, D. Tanaka, M. Nakashima, Y. Ooyama

721. Preparation of silica/hydrophilic polymer inorganic-organic hybrid oil/water separation membranes via sol-gel method. T. Tanaka, K. Kuraoka

722. Gas and water separation properties of acetoxy group-containing bridged polysilsesquioxane membrane. K. Yamamoto*, J. Ohshita, T. Tsuru

723. Preparation of imidazolium-group-containing cyclic siloxane indicating ionic liquid nature. T. Kubo*, S. Koge, J. Ohshita, Y. Kaneko

724. Synthesis and photo-induced electron injection process studies in a ruthenium containing triblock copolymer/multiwalled carbon nanotubes composite. H. Shi, L. Du, W. Chan, D.L. Phillips

725. Structure and properties of bacterial cellulose/nanofiller composites by in situ cultivation. R. NARAHARA, C. Hongo, T. NISHINO*

726. Preparation of organic-inorganic hybrid patterns by utilizing reaction development patterning. S. Imabayashi*, T. Oyama

727. Control of properties of composite films of conjugated polymers containing POSS fillers. K. Ueda*, K. Tanaka, Y. Chujo

728. Preparation and characteristics of ionic liquid containing cage-like oligosilsesquioxane with different types of side-chain groups. A. Harada*, S. Koge, J. Ohshita, Y. Kaneko

729. Sol-gel synthesis of amphiphilic silsesquioxane capable of forming reverse micelle. A. Nagatomo*, Y. Kaneko

730. Preparation of soluble polysilsesquioxane containing mercapto groups. H. Kugimiya*, Y. Kaneko

731. Preparation of ionic liquids containing cyclic siloxanes with ammonium side-chain groups. T. Hirohara, Y. Kaneko

732. Synthesis of thermoresponsive polysilsesquioxane containing urea group. S. Yamamoto*, Y. Miyasaka, Y. Kitamoto, O. Moriya

733. Control of thermoresponsibility on polysilsesquioxane having urea and fluorescent groups. Y. Kitamoto*, S. Yamamoto, O. Moriya

734. Fabrication of free-standing calcite thin films from octacarboxy-terminated T8-caged silsesquioxane-vaterite composite particles. S. Miyachi*, K. Naka, H. Imoto

735. Synthesis of π -conjugated units terminated polyhedral octasilsicate-core dendrimers and their material properties. Y. Irie*, S. Takata

736. Stepwise functionalization of polymer and material surface using orthogonal nitrile N-oxide agent. S. Cheawchan*, H. Sogawa, T. Takata

737. Gigantic enhanced circular dichroism of optically active di-alkylphenyl/polyisilanes during aggregation by limonene chirality transfer. K. Yoshida*, M. Fujiki

738. Luminescence supramolecular metalloge constructed by Pt(II) complex possessing bis(phenylisoxazolyl)phenylacetylene ligand. K. Hirano*, T. Haino*, T. Ikeda

739. Synthesis of the noncovalently-linked sequence-regulated polymers formed by molecular recognition. T. Hiroa*, T. Haino*

740. Hydrogel biosensor based on bacterial cellulose with MWNTs.

a.j. kzar/shammary*, z. shi, g. Yang

741. Preparation of anionic UV curing films containing dispersed titania particles and their application to self-cleaning materials. Y. Tachibana*, M. Furutani, K. Arimitsu*

742. In-situ generation method of diiodoaromatics: Syntheses and optical properties of organoarsenic compounds with arsole backbone. T. Kato, K. Naka

743. Synthesis of 9-arsafluorene-Pt(II) complexes and their solid-state luminescence. S. Tanaka*, T. Kato, H. Imoto, K. Naka

744. Rheological characterizations of time-dependent structure and phase evolutions in polymer-aided silver pastes. J. Jiang*, J. Liang, H. Yi, C. Hu, S. Chen

745. Ring-opening polymerization of necklace shaped inorganic polymers alternately bearing a POSS cage and siloxane chains. N. Katsuta*, M. Kunikata*, T. MATSUO, T. Ooba

746. Synthesis and characterization of titanium phosphonate clusters. R. Hayami*, S. Tsukuda, T. Gunji*

747. Individually aligned tubular ZnO nanostructures on solid substrates. G. Jeon, S. Lee, S. Yim, J. Kim*, S. Yang*

748. Preparation of anionic UV-cured coating films including scaly silica modified with base-amplifying groups. S. Sugioka*, K. Watanabe*, M. Furutani, K. Arimitsu*

749. Molecular design and synthesis of D- π -A pyranine dyes for photodynamic therapy. T. Enoki*, Y. Ooyama, J. Ohshita

750. Organic electronic sensors with organic/inorganic hybrid nanolayers. J. Seo*, C. Lee, M. Song, H. Kim, Y. Kim*

751. Synthesis of the side-chain type metal-ladithiolen polymer complexes. H. Sato*, S. Tsukuda, T. Gunji

752. Synthesis of novel one-dimensional platinum coordination polymers having poly(vinyl ether) pendants. M. Tanaka*, J. MOTOKANAGI, M. MINODA

753. Effect of organic/inorganic hybrid polymeric materials on the performance of organic transistors. C. Lee*, J. Seo, H. Kim, Y. Kim*

754. Design of low crystalline isobutyl-substituted T8-caged silsesquioxane derivatives by star-shaped architectures.

T. Yamanaka*, Y. Irie, H. Imoto, K. Naka

755. Synthesis of oligosiloxanes and derivatives. I. Abe*, S. Tsukuda, T. Gunji*

756. Role of organic/inorganic hybrid interfacial technology and materials for low-cost biomedical devices. H. Kim*, C. Lee, J. Seo, J. Jeong, M. Song, C. Ha, Y. Kim*

757. Preparation of platinum-supported mesoporous silica. H. Suzuki*, S. Tsukuda, T. Gunji, H. Momose

758. Synthesis and properties of cage octasilicate polymers. T. Igashii*, S. Tsukada, T. Gunji

Hawaii Convention Center
325A

Polymer Materials Performance, Degradation and Optimization (#369)

Organized by: M. Celina, T. Dargaville, H. Kudo, J. Lewicki
Presiding: B. Fayolle, H. Kudo

8:00 – 759. Applications of high-resolution X-ray CT to the characterization and quantitative analysis of physical and chemical aging in polymeric foam materials. J.P. Lewicki*, A. Maisano*, T. Weisgraber, A. Maiti, S.C. Chinn, T.S. Wilson, R.S. Maxwell

8:30 – 760. Tools for predicting radiation effects in silicone elastomers. S.C. Chinn*, R.S. Maxwell, J.P. Lewicki, T.S. Wilson, L. Dinh, A. Maiti, T. Weisgraber, W. Small

9:00 – 761. Enzymes that "eat" plastics: The search for true polyurethanes. A.L. Cockrell*, D.E. Barlow, W.J. Crookes-Goodson, J.N. Russell, J.C. Biffinger

9:30 – 762. Characterisation of transformation products of vitamin E in UHMWPE-based orthopaedic implants. S. Al-Malaike*

10:00 BREAK

10:10 – 763. Study on conductivity change of PEDOT/PPS by EB irradiation. T. Hinata, A. Oshima, M. Washio*

10:40 – 764. Major tunability of translational diffusivity of small molecules in thin polymer films: A confinement effect study. T. Lan, J. Torkelson*

11:10 – 765. Cure chemistry kinetics in epoxy materials. M.C. Celina*, N. Giron, A. Quintana

11:35 – 766. Can non-isothermal decomposition measurements be used to assess aging of polymers? J.G. Cordaro*, A.M. Kruizinga, A.S. Moore, A. Nissen

Hawaii Convention Center
323A

New Perspectives of Bioplastics for Environmental Benign Materials (#396)

Organized by: U. Hiroshi, I. Chin, T. Iwata, J. Li, P. Smith
Presiding: I. Chin, U. Hiroshi

8:00 – 767. Advances in microbial system for production of PLA-related polymers. S. Taguchi*

8:30 – 768. Biosynthesis and characterization of poly(3-hydroxybutyrate-co-3-hydroxyhexanoate) using oil and flower extract from *Madhuca indica* (Mahua). K. Sudesh*

9:00 – 769. Microbial synthesis of P(glycolate-co-3-hydroxybutyrate) with hydrolytic degradability. K. Matsumoto*, T. Shiba, Y. Hiraide, S. Taguchi

9:20 – 770. Syntheses and properties of novel alternating copolymers of 3-hydroxybutyrate and lactate units. H. Abe*

9:40 – 771. Development of metabolically engineered microorganisms for biobased sustainable production of bioplastics and monomers. S. Park*, Y. Oh, S. Lee

* Principle Author

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10:10 – 772. Innovative production of lactic acid from renewable resources for cost-effective production of biopolymers.
J. Wu*

10:40 – 773. Characterization and substrate specificity of a poly(lactate-co-3-hydroxybutyrate) depolymerase from soil bacterium. **C. Utsunomiya**, J. Sun, K. Matsumoto, T. Ooi, S. Taguchi*
11:00 – 774. Preparation of biodegradable polyester P(3HB-co-3HV) films prepared by aging on cold crystallization and by soaking solvent effect. **T. Tanaka***, T. Iwata

11:20 – 775. Antistaphylococcal, anti-Candida, and anti-influenza activities of poly- γ -glutamate-based supramolecular plastics-coated surfaces. **M. Ashiuchi***, S. Oike, S. Shibatani, H. Kubaka, N. Oka, H. Kobayashi, K. Yoneda

Hawaii Convention Center
327

Advances in Precision Polymer Synthesis Using Reversible Deactivation Radical Polymerization (#401)

Organized by: D. Keddie, N. Tsarevsky, G. Moad, S. Yamago
Presiding: D. Keddie, G. Moad

8:00 – 776. Organocatalyzed living radical polymerization controlled by photo irradiation. **A. Goto***

8:30 – 777. Precision polymer synthesis by combining light driven reactions with RDRP. **C. Barner-Kowollik***

9:00 – 778. Novel organocobalt based on acetylacetone ligands for the precision synthesis of telechelic polymers. **J. Demarteau***, D. Cordella, A. Kermagoret, A. Debugeine, C. Detrembleur

9:15 – 779. Phosphine-grafted RAFT-monomers as catalysts for Michael addition reactions in flow synthesis. **K. Barlow***, X. Hao, T. Hughes, O. Hutt, A. polyzos, K. Turner, G. Moad

9:30 – 780. RAFT of ethylene. **F. D'Agosto***, V. Montel, C. Domanguet, C. Boisson, S. Norsic

10:00 – 781. Access to ultra-high molar mass block copolymers by aqueous RAFT gel polymerization. L. Despax, S. Harrisson, E. Read, A. Cadix, J. Wilson, **M. Destarac***

10:30 – 782. Controlled radical photopolymerization of vinylidene fluoride and synthesis of PVDF block copolymers. **A. Asandei**

10:45 – 783. Exploring the capabilities of novel photochromic RAFT agents with photoswitchable reactivity. **O. Majewski***, D. Keddie, M.L. Coote, D.A. Lewis

11:00 – 784. Macromolecular engineering by organotellurium-mediated radical polymerization (TERP). **S. Yamago**

11:30 – 785. Nitroxide-mediated radical ring-opening copolymerization: A single cyclic ketene acetal comonomer to control the polymerization of methacrylates and to confer degradability. V. DELPLACE, S. Harrisson, Y. Guillaneuf, D. Gignes, **J. NICOLAS***

Hawaii Convention Center
325B

Aggregation Induced Emission: Materials and Applications (#444)

Organized by: M. Fujiki, B. Tang, B. Liu
Presiding: M. Fujiki, B. Liu, D. Zhang

8:00 – 786. Silole-based cyclosiloxanes with high solid-state fluorescence quantum yields and their AIE properties. **R. West***, Y. Cai, K. Samedov, B.Z. Tang

8:40 break

8:50 – 787. Photochemical properties of novel organoiron dendrimers. **A.S. Abd-El-Aziz**, A.A. Abdellghani, C. Agatemo, B. Thabet, S. Ahmed

9:20 – 788. Tuning the solid state packing and optical properties of organic crystals. **M. Hariharan***

9:50 – 789. Sensing and bioimaging agents incorporating AIE-active tetraaryl- and heteroarylethylenes. **F.C. Pigge**
10:20 break

10:30 – 790. Theranostic systems built via endowing responsive polymers with AIE features. **X. Wang, S. Liu***

11:00 – 791. Bioprosbes based on AIgen. **B. Liu***

11:20 – 792. Network polymers crosslinked by AIE molecules. **K. Kokado***, R. Taniguchi, K. Sada*

11:40 – 793. Design and syntheses of aminobenzopyranoxanthenes (ABPXs) with single-molecule multiple fluorescence emission and coloration. **S. Kamino**

Thursday Afternoon

Hawaii Convention Center
324

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madsen, K. Saalwachter, Y. Yao, J. Battiste
Presiding: H. Kaji, J.L. White

13:00 – 794. Monitoring spider silk assembly in vitro with NMR. **D. Xu, C. Guo, D. Onofrei, G.P. Holland**

13:25 – 795. Structure of *Bombyx mori* silk fibroin studied with NMR. **K. Okushita, T. ASAKURA**

13:50 – 796. NMR studies for the development of tissue-engineered cardiac patches based on silk fibroin.

Y. Nakazawa*, A. Asano, C.T. Nakazawa, T. Kameda, S. Nemoto, Y. TOMINAGA

14:15 – 797. Using NMR to elucidating the structure and dynamics in spider silks and related protein-based biopolymers. **J. Berger, B. Cherry**

14:40 Break

14:55 – 798. Untying the knots and tangled chains: NMR studies of elastin's cross-linking and hydrophobic domains.

K.K. Kumashiro

15:20 – 799. ^{13}C , ^2H NMR studies of structural and dynamical modifications of glucose exposed porcine aortic elastin. M. Silverstein, K. Bilici, S. Morgan, Y. Wang, Y. Zhang, **G. Boutis**

15:45 – 800. NMR study of the binding mechanism of peptides to metal oxide surfaces. **Y. Suzuki**

16:10 – 801. Characterization of gels from poly(allyl amine) and poly(ϵ -L-lysine) with carbon dioxide as gelant by solid NMR. **S. Maeda*, K. Kunimoto**

Hawaii Convention Center
325B

New Perspectives of Synthetic and Biological Soft Matter (#57)

Organized by: F. Horkay, J. Douglas, N. Choudhury, H. Jinnai
Presiding: H. Jinnai, R.A. Siegel

13:00 – 802. Dynamics of polyelectrolyte gels. **M. Muthukumar***

13:30 – 803. Molecular rigidity and entropy-enthalpy compensation in DNA hybridization. **J.F. Douglas, F. Vargas Lara**

14:00 – 804. Some new observations on poly(acrylic acid) gels. J. Scott-McKean, J. Garr, A. Walker, A. Costa, **G. Wnek***

14:30 Break

14:40 – 805. Cartilage extracellular matrix as a composite medium. **P. Bassar***, F. Horkay

15:10 – 806. Collective motion of active swimming particles analogous to acoustic wave propagation. **R. Yamamoto***, N. Oyama, J. Molina

15:40 – 807. Novel computational method for calculating electromagnetic and hydrodynamic properties of objects having arbitrary shape.

B.A. Pazmino Betancourt, J.F. Douglas

16:00 – 808. Factors controlling the directed self-assembly of microtubule nano-arrays. **M. Bachand, N. Bouxsein, S. Cheng, M. Stevens, G.D. Bachand**

16:20 – 809. Predictive computational approach for calculating the hydrodynamic solution properties of DNA-functionalized gold nanoparticles and other self-assembled DNA constructs. **F. Vargas Lara, J. Liddle, J.F. Douglas**

16:40 – 810. Single nucleotide polymorph analysis using toehold-mediated DNA strand displacement. **R. Fenati, D. Khodakov, A. Ellis***

Hawaii Convention Center
326A

Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158)

Organized by: T. Meyer, M. Ouchi, H. Steinman, Z. Li
Presiding: Z. Li

13:00 – 811. Precision glycomacromolecules – a chemist's approach to tune biointeractions. S. Igde, H. Wöhlk, C. Gerke, **L. Hartmann***

13:30 – 812. Translation and selection of functional sequence-defined synthetic polymers. **D.R. Liu**

14:00 – 813. Sequence-defined oligomers: Tuning structure and properties via sequence control. **C.A. Alabi***

14:30 Break

14:40 – 814. Exploiting sequence-dependent molecular recognition in the engineering of polymeric gels. **D.A. Tirrell***

15:10 – 815. Biomimetic sequence defined polymers based on a new backbone architecture: Synthesis and simulation.

J.W. Grate*, K. Mo, M. Daily, X. Ma, H. Jin

15:40 – 816. Peptide mimetic precision polymers: "Learning how to glue". **H. Boerner***, E. Maron

16:10 – 817. Effect of oligonucleotide sequence on thermal properties of a cross-linking ionic network. **K. Yang**, A. Coates, J.S. Moore*

Hawaii Convention Center
323C

Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194)

Organized by: K. Tanaka, A. Crosby, S. Kim, K. Dalnoki-Veress
Presiding: C.J. Ellison, S. Kim

13:00 – 818. Self-assembly of block copolymer particles. **G. Yi*, D. Jung, J. Oh, B. Kim**

13:30 – 819. Kinetics of the dynamic polymer brush formation at polymer water interfaces. H. Tanoue, M. Intusuka, K. Inoue, K. Ito, **H. Yokoyama***

13:45 – 820. Conformation of single polymer chain in spin-cast thin films revealed by super-resolution fluorescence microscopy. **H. Aoki***, T. Kuroda, T. Asada, T. Tanii

14:00 – 821. Programming surface energy driven Marangoni convection in polymer thin films to generate topographic patterns. **C.J. Ellison***, C. Kim, D. Janes, T. Arshad, R. Bonnecaze

14:15 – 822. Theoretical study of interfaces between ordered block copolymer phases. **A. Shi***

14:45 – 823. Segregation of chain ends to the surface of a polymer melt. **M.W. Matsen***, P. Mahmoudi

15:15 – 824. Toward an understanding of glass transitions in thin polymer films. T. Salez, J. Salez, K. Dalnoki-Veress, E. Raphael, **J. Forrest***

15:45 – 825. Heterogeneous and interfacial dynamics in stacked thin polymer films. **K. Fukao***, T. Hayashi, K. Sadakane, N. Yamada

16:00 – 826. Transition to area-dependent dissipation in droplet spreading. M. Ilton, O. Bäumchen, **K. Dalnoki-Veress**

16:15 – 827. Uniaxial stress-strain mechanics for ultrathin polymer film. **A.J. Crosby***, Y. Liu

16:30 – 828. Hydrodynamic slip: origins and effects in micro- and nanoscopic polymer flows. **J.D. McGraw***, K. Jacobs

Hawaii Convention Center
325A

Polymer Materials Performance, Degradation and Optimization (#369)

Organized by: M. Celina, T. Dargaville, H. Kudo, J. Lewicki
Presiding: J.P. Lewicki, J. Maisano

13:00 – 829. Radiation-induced synthesis of metal nanoparticles in ethers THF and PGMEA. **H. Yamamoto***

13:30 – 830. Evaluation of long-term stability and degradation on plastic glass based on polycarbonate. **M. Ito***, Y. Masuda, K. Nagai

13:55 – 831. Effect of pre-irradiation on thermal resistant properties of ethylene-propylene elastomer. **M. Ito***

14:25 – 832. Degradation of cable insulation materials around a research nuclear reactor. **H. Kudo***

14:55 BREAK

15:05 – 833. Influence of prepolymers on kinetic oxidation of epoxy networks. **E. Ernault***, E. Richard, B. Fayolle

15:35 – 834. Oxidatively degradable epoxy resin. **N. Kihara***, T. Oguri, Y. Shirai

16:00 – 835. Oxidative ageing of a polychloroprene elastomer. P. Le Gac, P. Davies, M.C. Celina, G. Roux, J. Verdu, **B. Fayolle***

Hawaii Convention Center
323A

New Perspectives of Bioplastics for Environmental Benign Materials (#396)

Organized by: U. Hiroshi, I. Chin, T. Iwata
Presiding: U. Hiroshi, T. Iwata

13:00 – 836. Effect of block length on the physical and structural properties of multi-stereoblock poly(lactic-acid)s. **H. Yamane***, Y.W. Widhianto, K. Masutani, Y. Kimura

13:30 – 837. How to improve the processing and mechanical properties of PLA. **Y. Wang***

14:00 – 838. Two-step surface functionalization of poly(L-lactic acid) films with enzymes. **A. Pellis**, E. Herrero Acero, H. Weber, M. Obersriebnig, R. Breinbauer, E. Srebotnik, G.M. Guebitz*

14:20 – 839. Expanding the thermal properties of bioplastics. **S.A. Miller***

14:40 – 840. Degradable plastics with low-temperature formability. **I. Taniguchi***, K. Masutani

15:00 – 841. Functional materials from bio-based furan polymers. **N. Yoshie***

15:30 – 842. High performance bio-based materials from polysaccharides. **T. Iwata***

16:00 – 843. Orientation birefringence of cellulose triacetate/xylan acetate blend. **S. Nobukawa**, Y. Enomoto-Rogers, T. Iwata, M. Yamaguchi

* Principle Author

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16:20 – 844. Elastic modulus of the crystalline regions of biobased polyesters.
S. LEE*, C. Hongo, T. NISHINO
16:40 – 845. Biobased LC polarylates showing polarimetry-controlled fluorescence. **T. Kaneko***, K. Kan

Hawaii Convention Center
327

Advances in Precision Polymer Synthesis Using Reversible Deactivation Radical Polymerization (#401)

Organized by: D. Keddie, N. Tsarevsky, G. Moad, S. Yamago
Presiding: N.V. Tsarevsky, S. Yamago

13:00 – 846. Transition metal-catalyzed living radical polymerization: Catalysis and catalyst design. **M. Sawamoto***

13:30 – 847. Approaches to RAFT synthesis of multifunctional, multi-armed polymers – the stars of therapeutic delivery.

G. Moad, K. Barlow, A. Postma, J. Chieffari, E. Rizzardo, J. Rosselgong, s. thang, X. Wei

14:00 – 848. Synthesis of functionalized amphiphilic block copolymers by RAFT to immobilize organocatalysts.

D. Kuckling*, X. Yu, A. Döring, M. Schneider, S. Pascual

14:15 – 849. Synthetic methodologies for polymer grafted nanoparticles via RAFT polymerization. T. Neely, M. Bell, **B.C. Benicewicz***

14:30 – 850. Organometallic mediated radical polymerization, a versatile tool for the precision synthesis of unprecedented copolymers. **C. Detrembleur**, D. Cordella, J. Demarteau, A. Kermagoret, N. Patil, C. Jérôme, A. Debuigne

15:00 – 851. Synthesis of high-precision polymers using radical oligomerization and polymerization. **J. Lutz***

15:30 – 852. Polymerization and degradation of aliphatic polyesters synthesized by atom transfer radical polyaddition.

C. Huang*, Y. Han, H. Chen

15:45 – 853. Visible-light organic photocatalysts for atom transfer radical polymerization. **G. Miyake**

16:00 – 854. Effect of scandium triflate on the RAFT copolymerization of methyl acrylate and vinyl acetate controlled by an acid/base "switchable" chain transfer agent. A. Tslepy, T. Schiller, S. Harrison, C. Guerrero-Sanchez, G. Moad, **D. Keddie***

16:30 – 855. Sulfur free RAFT polymerisation to methacrylic block copolymers in emulsion polymerisation. **D. Haddleton***

Hawaii Convention Center
323B

Aggregation Induced Emission: Materials and Applications (#444)

Organized by: M. Fujiki, B. Tang, B. Liu
Presiding: F.C. Pigge, H. TIAN, J. Yu

13:00 – 856. Design strategies and sensing protocols based on luminescent metal complexes via electrostatic assembly and aggregation processes. **V. Yam***

13:40 – 857. Color-tunable fluorescence based on the vibration induced emission of phenazine. **H. TIAN**

14:10 break

14:20 – 858. Pentacyclic coumarin-based blue emitters – the new case of AIEE. **D.T. Gryko**

14:50 – 859. Multicomponent and domino syntheses of AIE chromophores. **T.J. Müller***

15:10 – 860. Ultrasound-induced transformation of fluorescent organic nanoparticles from a molecular rotor into rhomboidal nanocrystals with enhanced emission. **D.M. Guidi**

15:40 break

15:50 – 861. Aggregation induced near infrared emission. **A. D'Aléo***, E. Zaborova, F. Fages

16:10 – 862. Trigonal azobenzene assembly into 1D structures with aggregation-induced emission enhancement characteristics. **M. Han***, S. Cho, Y. Norikane, M. Shimizu, A. Kimura, T. Tamagawa, Y. Takeoka, T. Seki

16:30 – 863. Twisted luminescent molecules for solar concentration. **K. Ghiggino***, J. Banal, W. Wong

16:50 – 864. AIE based water-soluble nano-fluorogens for the application in cell imaging. Y. Xia, Y. Jin, **B. Song***

17:10 – 865. Structure-property correlations and functional opportunities of AIE active organic/organometallic luminogens. **T. Pakkirisamy***

Thursday Evening

Hawaii Convention Center
324

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madsen, K. Saalwachter, Y. Yao, J. Battiste

Presiding: A. Whittaker

19:00 – 866. NMR imaging in the study of drug tablets in simulated biological fluids. E. Assad, Y. Wang, M. Mateescu, **J.X. Zhu***

19:25 – 867. Shear banding and spatio-temporal fluctuations in complex fluids investigated by advanced Rheo-NMR.

S. Kuczera, T.I. Brox, B. Douglass, M.A. Williams, **P. Galvosas***

19:50 – 868. Field-cycling NMR: From simple relaxometry to molecular rheology. **E. Roessler***, M. Hofmann, F. Fujara, B. Kresse, A. Privalov, N. Fatkuljin

20:15 – 869. Ultrafast sample spinning for solid-state NMR. M.K. Pandey, M. Malon, J.R. Yarava, A. Ramamoorthy, **Y. Nishiyama***

Hawaii Convention Center
Halls I, II, III

New Perspectives of Synthetic and Biological Soft Matter (#57)

Organized by: F. Horkay, J. Douglas, N. Choudhury, H. Jinnai
Presiding: J.F. Douglas, F. Horkay

Poster Session

19:00 – 21:00

870. Effective tracheal tissue regeneration by bioactive molecules-loaded asymmetrically porous matrix. S. Lee, T. Kim, S. Oh, S. Kwon, **J. Lee***

871. Peripheral nerve regeneration through asymmetrically porous nerve guide conduit with nerve growth factor gradient. T. Kim, J. Kang, S. Oh, **J. Lee***

872. Acid-cleavable PEO-*b*-PPO-*b*-PEO copolymers as "smart" surfactants for mini-emulsion polymerization. **M. Worm***, H. Frey

873. Preparation and characterization of polyampholyte copolymers of *N*-(3-aminopropyl) methacrylamido hydrochloride (APM) and acrylic acid (AA). **J. Zhao**, N. Burke, H.D. Stöver*

874. Preparation of amylose supramolecular gel materials by vine-twining polymerization. **K. Tanaka**, D. Hatanaka, K. Yamamoto, J. Kadokawa*

875. Cartilage: Supramolecular structure and biological function. **F. Horkay***, I. Horayne-Szakaly, E.K. Dimitriadis, P. Basser

876. Visualization of hierarchical structure in hydrogel of self-assembled synthetic polypeptide. **K. Yamamoto***, E. Ito, H. Yokoi, A. Otani

877. Preparation of cellulosic nanofiber and its application in polymer films. **J. Kim***, K. Son, S. Jang

878. Photolysis of self-assembled monolayers and model compound using photodegradable 2-nitrophenethyl linker. **M. Ito**, K. Yamaguchi

879. Assembly and functionalization of nano-objects from polymer-grafted proteins. **K. Fujimoto***, Y. Fukui

880. Structural and property development of silicone elastomer blended with crystalline component. **Y. Isogai**, H. Uehara, T. Yamano, E. Akiyama

881. Comparative study on phase behavior of AB diblock copolymer, cyclic AB diblock copolymer, and ABA triblock copolymer. **Y. Jeong***, T. Chang

Hawaii Convention Center

326A

Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158)

Organized by: T. Meyer, M. Ouchi, H. Sleiman, Z. Li
Presiding: J. Lutz

19:00 – 882. Precision polymer constructs for next-generation biodegradable polymer-drug conjugates. **M.F. Ebbesen***, A. Banger, L. Cappel, C. Gerke, L. Hartmann

19:30 – 883. Sequence-controlled vinyl polymers from bulky and cleavable monomers. **D. Oh**, M. Ouchi*, M. Sawamoto*

20:00 – 884. Synthesis and electrochemical characterization of oligonucleotide-inspired organic nanowires.

A. Mazaheri-pour*, N. Husken, J. Jocson, A. Burke, **A.A. Gorodetsky**

Hawaii Convention Center
Halls I, II, III

Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194)

Organized by: K. Tanaka, A. Crosby, S. Kim, K. Dalnoki-Veress

Poster Session

19:00 – 21:00

885. Molecular interaction between polymers and low-molecular weight compounds 19: Identification of poly(amine acids). H. Kanazawa, **A. Inada**

886. Synthesis of highly surface active amphiphilic chitosan nanoparticles. a.m. **atta**, h.a. **al-hoqedan**

887. Synthesis of novel polymers having precisely placed tetrahydrofurfuryl side-chain branches via regio/stereoselective ring-opening metathesis polymerization. **M. Kataoka**, S. Kobayashi, R. Satou, M. Tanaka*

888. Synthesis amphiphilic polylonic liquid based on 2-acrylamido-trimethyl ammonium salt as petroleum crude oil additives. a.m. **atta**, h.a. **al-hoqedan**

889. Synthesis of composite particles by seeded emulsion polymerization with microgel particles as seeds. **T. Watanabe**, C. Kobayashi, T. Kureha, D. Suzuki*

890. Novel and facile method to synthesize hollow cyanocrylate nanoparticles. **T. Matsubayashi**, M. Tenjimbayashi, K. Manabe, S. Shiratori

891. Repeatable adhesion using a hydrogen-bonding interaction of poly(4-vinylpyridine) brushes. **H. Yoshioka***, K. Yamaguchi, M. Kobayashi

892. Photopolymerization-induced surface segregation of zwitterion polymers in superhydrophilic protective coating. **M. Kobayashi**, T. Suga, H. Nishide*

893. In-situ formation of nano-scaled surface feature during photocuring: Design of functional block copolymer additives. **K. Katayama**, K. Minamibayashi, T. Suga, H. Nishide*

894. One-step preparation of core-shell polyacrylate latex containing fluorine and silicone and its film properties. **T. Lyu***, H. Zhao, D. Zhang

895. Simultaneous control over size, shape, and nanostructure of monodisperse block copolymer colloidal particles. **J. Shin**, H. Hwang, B. Kim*

896. Structural characterization of poly(*N*-isopropylacrylamide-co-ruthenium tris(2,2'-bipyridine)) microgel investigated by small-angle X-ray scattering.

S. Matsui, T. Kureha, Y. Nagase, K. Okeyoshi, R. Yoshida, T. Sato, D. Suzuki*

897. Structure analysis of N-linked glycan of laccase from Japanese lacquer tree.

O. TUMURBAATAR, T. Yoshida

898. Effect of alignment layers on molecular alignment induced by photopolymerization. **M. Ishizu**, K. Hisano, A. Shishido*

899. Colloidal crystals from Poly(vinylidene fluoride) nanospheres. **D. OKADA***, S. Furumi, M. Takeguchi, Y. Yamamoto

900. Interfacial structure of poly(methyl methacrylate) stereocomplex. **K. Sasahara**, M. Inutsuka, A. Horinouchi, K. Tanaka*

901. Self-assembly polymer brush via surface segregation of liquid crystalline block copolymer in the bulk and thin film states. **S. Nojima**, Y. Higaki, R. Ishige, M. Kido, T. Hirai, A. Takahara*

903. Interfacial effects on the crystallization and surface properties of poly(L-lactic acid) ultrathin films. **A. Udagawa***, T. Fujie, Y. Kawamoto, A. Saito, S. Takeoka, T. ASAHI*

904. Primer effect on adhesion and microstructure of isotactic polypropylene/cyanacrylate interface. **Y. NAKANISHI**, C. Hongo, T. NISHINO

905. Lattice deformation of microphase separated structure in diblock copolymer thin film revealed by low energy. **I. Saito***, K. Yamamoto

906. Nanopatterning with block copolymer with strong segregation. **H. Mitsushima**, M. Takenaka

907. Perpendicular oriented lamellar nanostructures with sub-10 nm features by surface segregating fluorine- and silicon-containing block copolymers. **T. Hayakawa***, H. Takanishi, L. Wang, Y. Tanaka, R. Maeda

908. Microphase-separated structures in block copolymer droplets prepared by solvent-induced dewetting. **Y. Hirai***, T. Higuchi, H. Jinnai, H. Yabu

909. Restraining factor in ionic conductivity: The role of interphase in semicrystalline poly(ethylene oxide)/LiClO₄ electrolyte. **X. Zhang***, Y. Wang, H. Ye, Q. Zhou

910. Polymer nanotubes confined to cylindrical alumina nanopores: Tailoring tube thickness and Tg. **A.W. Tan***, J. Torkelson

911. Search for a fluorescence probe with thermal stability to examine interfacial polymer mobility. **M. Aoki**, D. Kawaguchi, T. Ganbe, N. Sekine, K. Okamoto, K. Tanaka*

912. Substantial spatial heterogeneity and tunability of glass transition temperature observed with dense polymer brushes prepared by ARGET ATRP. **T. Lan**, J. Torkelson

913. Glass transition and dynamics of PS/P2CS/PS stacked thin films. **K. Suzuki**, N. Taniguchi, T. Hayashi, K. Sadakane, K. Fukao

* Principle Author

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- 914.** Different glass transition behavior of confined polystyrene thin films supported on graphitic vs. silica substrates.
L. Chen, J. Torkelson*
- 915.** Dielectric relaxation behavior of thin films of polyamide random copolymers.
N. Taniguchi, K. Fukao
- 916.** Study of surface analysis of polystyrene nano particle by using attenuated total reflectance spectroscopy in the far-UV region.
Y. Morisawa, T. Ochi
- 917.** Study of magnetic thermoplastic elastomers with enhanced mechanical properties.
F. Jiang, J. Bai, Z. Wang*
- 918.** Thermal adhesion property of polystyrene brushes.
Y. Aoki*, K. Yamaguchi, M. Kobayashi
- 919.** Modification of chemically stable polymeric materials 60: Improvement in the adhesive property of polymeric and FRP materials.
H. Kanazawa, **T. Tanaka**, A. Inada, T. Ara
- 920.** Molecular simulations of lubrication properties of concentrated polymer brushes.
H. Okamoto*, T. Koga
- 921.** Effects of the interfacial reaction on morphology and toughness of polyamide 6 blends with ethylene copolymers carrying different reactive groups.
E. Yamada*, H.T. Oyama, K. Uetani, Y. Mori
- 922.** Fabrication of large-area microstructures for superhydrophobic surfaces using screen-mesh architectures.
H. Tokuhisa, S. Tsukamoto, S. Morita, N. Shirakawa
- 923.** Study of electronic state of polyethylene glycol with attenuated total reflectance spectroscopy in far ultraviolet.
N. Ueno, Y. Morisawa
- 924.** Tuning mechanical and optoelectrical properties of poly(3-hexylthiophene) through systematic regioregularity control.
J. Kim, J. Kim, W. Lee, H. Yu, H. Kim, I. Song, M. Shin, J. Oh, U. Jeong, T. Kim*, B. Kim*
- 925.** Hydration and viscoelasticity measurements of biocompatible polymers by using quartz-crystal microbalance with energy dissipation technique.
S. Xue, S. Kobayashi, M. Tanaka, H. Furusawa*
- 926.** Investigation of the mechanism underlying biointeraction of self-assembled monolayers by surface force measurements.
T. Sekine*, M. Tanaka, C. Sato, A. Tsunoi, T. Yano, M. Hara, T. Hayashi*
- 927.** Preparation of liquid crystalline polymer films with chromophores and their fluorescent behaviors.
K. Ueda, A. Kawamura, T. Miyata*
- 928.** Preparation of smart films exhibiting structural color by assembling stimuli-responsive gel particles.
Y. Nishimura, A. Kawamura, T. Miyata
- 929.** Direct and vapor contact antifungal activity assays of essential oils impregnated in nanocellulose reinforced chitosan, poly lactic acid, and methyl cellulose composite films.
F.M. Hossain*
- 930.** Cellular behavior on polymer scaffolds with 2D-pattern of mechanical properties.
S. Shimomura, K. Sanada, H. Matsuno, Y. Kinoshita, S. Fujimura, K. Tanaka*
- 931.** Plasma modification of carbon-steel surface for improving green elastomeric blend adhesion.
J. Oravec*, J. Preto, J. Hronkovic, P. Melus, H. Hirahara, J. Sang, S. Aisawa, K. Miura
- 932.** Electrophoretic mechanism of non-ionic poly(ester-sulfone)s.
M. Yokoyama, A. Takasu
- 933.** Preparation of porous Poly(pyrrrole) utilizing agar particles as soft template and evaluation of its actuation property.
S. Tamesue*, K. Obata, T. Mitsumata, N. Tsubokawa, T. Yamauchi
- 934.** Controllable end group modification of PAMAM and its study on the stability mechanism of immobilized AChE.
H. Liu, J. Diao, Y. Sun
- 935.** Identification and characterization of peptides that recognize stereoregular poly(*N*-isopropylacrylamide).
S. Suzuki, T. Sawada, T. Ishizone, T. Serizawa*
- 936.** Multi-chromic polymer nanoparticles composed of a polythiophene derivative in aqueous media.
K. Salikolimi, P. He, Z. Li, T. Aigaki, Y. Ito, M. Kawamoto

- 937.** Transparent rapidly liquid slipping smooth surface with self-healing property.
M. Tenjimbayashi, T. Matsubayashi, K. Manabe, S. Shiratori*
- 938.** Evaluation of interaction for bioactive compounds with thermoresponsive polymer brush grafted on polystyrene monolith surfaces using capillary chromatography.
T. Koriyama, T. ASOH, R. ISHIHARA, A. Kikuchi*
- 939.** Synthesis of polyamine block copolymers for removal of engineered nanopollutants from water.
R.F. DSouza, S. Valiyaveettil*
- 940.** Antifouling flat film with transparency, self-standing, and flexible property.
T. Nakashima*, M. Tenjimbayashi, K. Manabe, S. Shiratori, M. Fujita, T. Kamiya, T. Honda
- 941.** Antibiofouling surface with plant oil infused porous structure for laparoscope lenses.
S. Nishioka, M. Tenjimbayashi, K. Tsukada, S. Shiratori
- 942.** Photo-activation bonding between polymer material and aluminum.
C. Kong*, T. Utsunomiya, T. Ichii, H. Sugimura
- 943.** Flexible cotton fabrics with reversible wettability.
K. Sasaki, M. Tenjimbayashi, K. Manabe, S. Shiratori
- 944.** Clay/polymer composite with water vapor barrier property by spray layer-by-layer assembly method.
M. Notoya, K. Kyung, K. Fujimoto, S. Shiratori
- 945.** Effect of micro-roughness of interface on adhesion strength of aluminum/polymer joint.
D. Seo, S. Lee, C. Lee, J. Seo, J. Jho*
- 946.** Organosilane molecular film formation on cyclo-olefin polymer surface for protective coating against organic solvents.
T. Utsunomiya, T. Kanzawa, K. Onishi, T. Ichii, H. Sugimura
- 947.** Introduction of microscale roughness onto polymer surface by replicating etched steel surface.
S. Lee, D. Seo, C. Lee, J. Seo, J. Jho*
- 948.** Molecular orientation control by crystal nucleating agent and healing property of craze phase.
A. Takeno*, Y. Horiguchi, T. Miyata, S. Takahashi
- 949.** Suppression of coffee-stain for Nafion thin film by ethanol vapor treatment.
Y. Ono, Y. Guo, Y. Nagao*
- 950.** Natural rubber latex with low protein and application.
N.T. Phan*, Y. Yoshimasa , S. Kawahara
- Hawaii Convention Center
Halls I, II, III
- New Perspectives of Bioplastics for Environmental Benign Materials (#396)**
- Organized by:* U. Hiroshi, I. Chin,
T. Iwata, J. Li, P. Smith
Presiding: U. Hiroshi
- Poster Session**
19:00 – 21:00
- 951.** Biosynthesis of unusual bioplastic: Medium chain length homo polyhydroxyl-kanoate from plant biomass.
A. HIROE*, K. MAEZIMA, S. WATANABE, T. Tsuge*
- 952.** Terminal modification of PVA via alcoholsysis reaction catalyzed by class IV synthase.
M. Hyakutake*, S. Tomizawa, K. Mizuno, T. Tsuge, H. Abe
- 953.** Synthesis of polyhydroxylkanoates by photosynthetic purple bacteria.
M. Higuchi-Takeuchi*, **K. Numata**
- 954.** Biosynthesis and thermal characterization of novel microbial polyester bearing phenyl and phenylalkyl side groups.
S. Mizuno, T. Tsuge
- 955.** Substrate stereoselectivity of poly(Asp) hydrolase-1 capable of cleaving β -amide bond.
T. Hiraishi*, H. Abe, M. Maeda
- 956.** Preparation of bacterial cellulose/polyacrylonitrile composite monolith and its application for electrode of EDLC.
A. Dobashi, S. Kuwabata, J. Maruyama, U. Hiroshi
- 957.** Development of flame retardant polymer materials using ligninphenol derived from woody resource.
A. Nodera*, M. Funaoka
- 958.** Electromagnetic wave shielding effect of plastic/bamboo/graphite composites.
M. Maeda*, H. Nishida
- 959.** Sequential refining and utilization of lignin, molecular segments complex.
M. Funaoka*
- 960.** Temperature dependence of the elastic modulus of the crystalline regions of collagen triple helix.
S. Konoike, C. Hongo, T. NISHINO*
- 961.** Preparation of chitin nanofiber-based composite materials by surface modification.
R. Endo, K. Yamamoto, J. Kadokawa*
- 962.** Nucleating effect of xylan propionate on poly(lactide) stereocomplex.
D. Ishii*, M. Kimishima, K. Otake, T. Iwata
- 963.** Synthesis of star-shape biopolymers with extremely small branches and their application phthalate-free plasticizer designed for non-toxicity and improved migration resistance.
J. Chung*
- 964.** Impact modification of PLA by poly(*n*-butyl acrylate-g-*l*-lactide) with annealing induced intermolecular crystallization effect.
H. Lee, S. Kim, I. Chin*
- 965.** Generation of monolithic porous poly(lactic acid) with stereocomplex formation.
T. Kanno, H.T. Oyama, U. Hiroshi
- 966.** Synthesis and characterization of stereoblock polylactides consisting of L- and D-lactyl segments.
K. Masutani*, M. Yamamoto, Y. Kimura, H. Yamane
- 967.** Preparation and characterization of bio-based poly(crotonates) from the non-edible biomass.
Y. Takenaka*, H. Abe
- 968.** Synthesis of a series of vanillin-based polyesters and determination of their physical property.
K. Tachibana, H. Abe*
- 969.** Polyurethane elastomers based on a non-edible plant oil.
T. Kasahara, U. Hiroshi
- 970.** Development of biobased epoxy polymers derived from cashew nut shell liquid.
S. Kanehashi*, T. Miyakoshi
- 971.** Enzymatic polymerization of biobased catechol inspired oriental lacquer, "Urushi".
S. Kanehashi*, T. Miyakoshi
- 972.** Controlled/living cationic polymerization of vinyl ethers derived from glycerol.
A. Kajita, K. Satoh*, M. Kamigaito*
- 973.** Living radical polymerization of renewable styrene derivatives from natural resource.
H. Takeshima, K. Satoh*, M. Kamigaito*

Hawaii Convention Center
323B

Aggregation Induced Emission: Materials and Applications (#444)

Organized by: M. Fujiki, B. Tang, B. Liu
Presiding: Y. Hong, J. Xu

19:00 – 980. BODIPY-containing probe for cell-type-specific fluorescence imaging of plasma membrane, nucleus and/or nuclear envelope in live cells.
D. Chen, S. Gu, X. Feng, P. Liu, J. Shi, B. Tong, Y. Dong*

19:20 – 981. AIE behavior of tetraaryl-1,3-butadiene derivatives and their applications in mechanochromism, thermochromism, and explosive detection.
X. Feng, Y. Dong, B. Wang

19:40 – 982. Smart fluorescent dye with aggregation-induced emission characteristic for lysosome imaging and nucleic acid detection.
Y. Zhao, J. W. Y. Lam, B. Tang*

20:00 – 983. Emerging optically active luminescent poly(diptyfluorene) aggregates by polymer chirality transfer with helical polysilanes.
N. Abdul Rahim, S. Guo, N. Suzuki, M. Fujiki

20:20 – 984. Pentaphenylpyrrole derivatives with aggregation-induced emission characteristics as "turn-on" sensors for the detection of bovine serum albumin and metal ions.
B. Tong

20:40 – 985. Multicomponent tandem polymerizations towards functional conjugated polymers with aggregation-enhanced emission characteristics.
H. Deng, J. W. Y. Lam, B. Tang*

Friday Morning

Hawaii Convention Center
324

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madsen, K. Saalwachter, Y. Yao, J. Battiste
Presiding: L.A. Madsen, K. Saalwaechter

8:00 – 986. Stokes-Einstein and beyond: NMR studies of macromolecular diffusion in confined-bulk and crowded-solution environments.
K. Saalwachter

8:25 – 987. ^{31}P CODEX NMR and phospholipid lateral diffusion in membranes.
P.M. Macdonald*, Q. Saleem, A. Lai

8:50 – 988. HRMAS NMR pulsed field gradient diffusion investigations in soft and swollen materials.
T.M. Alam*

9:15 – 989. NMR spectroscopy, relaxometry, and diffusion studies of carbohydrates in ionic liquids.
M.E. Ries*, T. Budtova, S.M. Green, A. Radhi

9:40 Break

9:55 – 990. Influence of entanglements on chain diffusion and mechanical deformation in solid state of linear ultra high molecular weight polyethylene.
S. Rastogi*, S. Ronca, D. Romano, Y. Yao

10:20 – 991. Dynamics of random poly(styrene-co-methyl methacrylate) in bulk and on silica.
M. Maddumaarachchi, F.D. Blum*

* Principle Author

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10:45 – 992. How molecular dynamics contributes to the mechanical properties of elastomers and fibers. **W. Hu***
11:10 – 993. Segmental motions and hydrogen bond dynamics in supramolecular polymer-based architectures: A multinuclear solid-state NMR investigation. **C. Lorthioir***, J. Cortese, C. Soulié-Ziakovic

Hawaii Convention Center
325B

New Perspectives of Synthetic and Biological Soft Matter (#57)

Organized by: F. Horkay, J. Douglas, N. Choudhury, H. Jinna
Presiding: F. Horkay, M. Muthukumar

8:00 Opening Remarks

8:05 – 994. Nature-inspired hydrogels that change shape in response to external stimuli or to specific biomolecules. **S.R. Raghavan**

8:35 – 995. Sensing the surface: What can polymer brushes tell us about surface interactions? **K.L. Beers***, S. Orski, C. Deodhar, R. Sheridan
9:05 – 996. 3D shape (rod to corkscrew) transitions in thermosensitive hydrogels induced by a spiral scaffold. **R.A. Siegel***, H. Lee, J. O'Neill, T.M. Kowalewski

9:35 – 997. Directing order and functionality in stimuli-responsive intrinsically disordered protein polymer. **N.K. Dutta***, R. Balu, N. Roy Choudhury, C.M. Elvin, A.J. Hill

10:05 Break

10:20 – 998. Molecular positioning of nature's elastic assembly modules to build complex multidimensional vascular and microvascular structures. **A.S. Weiss***

10:50 – 999. Characterization of DNA/polymer nanoparticle and application for cancer immunotherapy. **J. Lisziewicz**, E.R. Toke, O. Lorincz, L. Molnar, Z. Csizsovszki, E. Somogyi, J. Toth, K. Pantya, J.F. Douglas, F. Horkay, F. Lori

11:20 – 1000. Preparation of poly(vinyl alcohol) hydrogels by γ -irradiation for cluster culture of neural stem cells. **H. Mori**, M. Hara

11:40 – 1001. Smart hydrogels based on DNA quadruplexes. **A. Kuzyua***, S. Tanaka, K. Wakabayashi, K. Fukushima, Y. Ohya

Hawaii Convention Center
Halls I, II, III

New Frontiers in Polymer Crystallization (#96)

Organized by: W. Hu, A. Toda, C. Li

Poster Session

10:00 – 12:00

1002. Imaging and controlling block copolymers crystallization using AFM. **L. Alarbe**

1003. Crystallization kinetics of polyethylene on fast cooling up to 10 MK/s. **E. Zhuravlev***, C. Schick

1004. Preparation of high-performance poly(oxyethylene) film by drawing techniques. **T. Sakamura**, H. Uehara, T. Yamanobe, T. Ikeda

1005. Single molecule study of polymer interactions in the single crystal of nylon-66. **X. Lyu**, W. Zhang*

1006. PS blocks improve the mechanical stability of the PS-b-PEO-b-PS single crystal. **P. Yang***, Y. Song, W. Zhang

1007. Aggregation structure of polyimide fibers during heat-drawing process. **Q. Zhang**, J. dong, C. Yin

1008. Thermodynamics of strain-induced polymer crystallization in solutions. **L. Zha**, W. Hu

1009. Molecular simulation of polymer crystallization in stereo-complex blends. **R. Zhang**, W. Hu

1010. Chain-length effects on the crystallization of cyclic polymers. **H. Gao**, C. Luo, W. Hu, J. Sommer

1011. Acceleration effect of retraction on strain-induced copolymer crystallization. **X. Guan**

1012. Designing of polymer crystallization nucleating agents: Synthesis and microstructure of polystyrene-block-poly(styrene-*aft*-maleic anhydride) block copolymers and their ionomers. **J. Si***, S. Xing, P. Tang

1013. Determination of local packing and chain folding structure of mesomorphic form isotactic polypropylene. **S. Yuan**, T. Miyoshi

1014. Crystallization and thermal behavior of Poly(ϵ -caprolactone) and its copolymers studied by vibrational spectroscopy. **T. Toyouchi***, H. Sato, Y. Ozaki

1015. Extraordinary phase transition observed in the helix-sense inversion of polyaspartate in the solid state. **y. suzuki***, H. Furuya, A. Abe

1016. Hydrogen bondings and stereocomplex formation of poly(L-lactic acid) and poly(D-lactic acid) during isothermal crystallization studied by Raman spectroscopy and X-ray diffraction. **H. Sato***, Y. Narihisa, D. Furukawa, Y. Ozaki

1017. Crystallization and chain orientation in the ultrathin films of poly(3-hydroxybutyrate) studied by IR-RAS and GIXD. **. Khasanah***, R. Kummetha, I. Takahashi, H. Sato, Y. Ozaki

1018. In-situ analysis for melt drawing behaviors of metallocene- and Ziegler-catalyzed ultra-high molecular weight polyethylene. **C. Narita***, H. Uehara, T. Yamanobe, K. Inatomi, S. Abe

1019. Acceleration in crystallization kinetics of polyalactide in immiscible blends through the comb-like copolymer strategy. **Y. ZHANG**, J. Wang, Z. WANG*

1020. Shear flow induced formations of shish-kebab and transcrystallite assisted with preformed spherulites in isotactic polypropylene. **J. Wang**, Y. ZHANG, Z. WANG*

1021. Shear-induced enhancements of crystallization kinetics and crystalline morphological evolutions for long chain branched polyalactides with different branching degree. **J. Wang**, J. Bai, Z. WANG*

1022. Shear-induced crystallization kinetics for asymmetric PLLA/PDLA blends. **J. Bai**, J. Wang, Z. WANG*

1023. Phase transition of isotactic polypropylene induced by heat-stretching. **T. Imai***, K. Yamada, K. Nozaki

1024. Electrospinning of Poly(vinylidene fluoride)-partially sulfonated Poly(1,4-phenylene sulfide) blends and their piezoelectric properties. **S. Pervin**, M. Yoo*, A. Prabu, K. Kim*

1025. Characterization of thin films of biodegradable $\text{P}(\text{HB-co-HX})/\text{PEG}$ blends. Y. Chen, Y. Park, I. Noda, Y. Jung

1026. Effects of molecular dynamics and crystallization kinetics on the mechanical properties and the structure of the amorphous phase of poly(ϵ -caprolactone). **A. Seidlitz***, Y. Men, T. Thurn-Albrecht

1027. Structure and physical properties of polymer/cyclodextrin composite: Poly(lactic acid) and polypropylene. **Y. Takada***, H. Uehara, T. Yamanobe, K. Takahashi

1028. Structural insights into the solid-state formation of the carbazolyl-diacetylene PDCH polymer. **B. Bagautdinov***, K. Sugimoto, H. Tanaka, S. SASAKI, K. Tashiro, M. Takata

1029. Microscopic kinetics model for nucleation of polymer crystallization. **J. Xu**

1030. Crystallization behavior of aliphatic polyesters with dialkene fumarate randomly copolymerized on main chain. **H. Ye***, C. Wang, Y. Song

1031. Crystalline structure control of poly(vinylidene fluoride) in antisolvent addition crystallization. **T. Nishiyama***, T. Sumihara, E. Sato, H. Horibe

1032. Non-solvent preparation of nanostructured membranes of ultrahigh molecular weight polyethylene by drawing technique. **H. Uehara***, T. Yamanobe

1033. FTIR spectroscopic analysis of the crystallization of precision halogen substituted polyethylenes. **X. Zhang**, L. Santona-Blasco, R.G. Alamo

Hawaii Convention Center
326A

Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158)

Organized by: T. Meyer, M. Ouchi,

H. Sleiman, Z. Li

Presiding: M. Ouchi

8:00 – 1034. Toward sequence control in homogeneous polymerization via single monomer addition in living ring-opening metathesis polymerization. **Y. Xia***

8:30 – 1035. Control of sequence for vinyl copolymers using bond manipulation. **M. Ouchi**

9:00 – 1036. Sequence control in RAFT polymerization. **G. Moad***, M. Danial, C. Guerrero-Sanchez, J. Haven, M. Hendrikx, A. Postma

9:30 – 1037. Sequence-controlled polymers via tandem catalysis of living radical polymerization and transesterification: Modular synthetic approaches to gradient and pinpoint functionalization. **T. Terashima**, M. Sawamoto

10:00 Break

10:10 – 1038. Monomer sequence control in main- and side-chains of vinyl polymers by controlled radical polymerization. **M. Kamigaito***, K. Satoh

10:40 – 1039. Precision polymers toward biological precision: Multiblock copolymers and monodisperse sequence-controlled oligomers. **T. Junkers**, J. Vandenbergh

11:10 – 1040. Preparation of 1:1 alternating, nucleobase-containing copolymers for use in sequence-controlled polymerization. **E.G. Williams***, s. thang, B. Fairbanks, R. Mulder, E. Rizzardo, G. Moad

Hawaii Convention Center
323C

Polymer Interfaces: Design, Structure, Physical Properties and Applications (#194)

Organized by: K. Tanaka, A. Crosby, S. Kim, K. Dalnoki-Veress

Presiding: K. Dalnoki-Veress,

R.D. Priestley

8:00 – 1041. Nanoconfinement of polymers in coordination nanochannels. **T. Uemura***

8:30 – 1042. Polystyrene nanoparticles and films: Identical glass transition temperature confinement effect through qualitative comparison. **L. Chen**, M. Szymusiak, Y. Liu, J. Torkelson*

8:45 – 1043. Enhanced Tg-confinement effect and related physical aging behavior in crosslinked polystyrene characterized by ellipsometry. **K. Jin**, J. Torkelson*

9:00 – 1044. Engineering structure and properties in polymer thin films by MAPLE. **R.D. Priestley**

9:15 – 1045. Inhibition of bacteria adhesion and protein adsorption on hydroxyapatite surface using PEG-Phosmer copolymers. **X. Cui**, Y. Kojima, H. Seto, Y. Hoshino, Y. Miura*

9:30 – 1046. Ion transport properties of block copolymer electrolytes: Effects of confinement and interface. **M. Park***

10:00 – 1047. Controlled growth of organic semiconductors by eutectic solidification. **Y. Kang**

10:30 – 1048. Flow field penetration into thin nanoporous polymer films under laminar flow by Förster resonance energy transfer coupled with total internal reflectance fluorescence microscopy. **J.E. Pemberton**, H. Wang, L. Cheng, E. Saez

10:45 – 1049. Catheter coatings for reduced bacterial growth. **V. Thompson**, D.B. Usuttate, P. Adamson, D. Gordon, I. Kooper*

11:00 – 1050. Design of molecularly imprinted polypeptide gel films on sensor chips and their target molecule-responsive behavior. **K. Matsumoto**, B.D. Tiu, A. Kawamura, R. Advincula, T. Miyata

11:15 – 1051. Morphology observation of natural rubber with nanomatrix structure. **L. Fukuhara**, S. Kawahara*

11:30 – 1052. High-performance all-polymer solar cells based on face-on stacked polymer blends with low interfacial tension. **B. Kim**

Hawaii Convention Center
325A

Polymer Materials Performance, Degradation and Optimization (#369)

Organized by: M. Celina, T. Dargaville, H. Kudo, J. Lewicki

Presiding: S. Al-Malaika, S.C. Chinn

8:00 Delayed start

8:10 – 1053. Synthesis of novel liquid-type latent curing agents to generate imidazoles and their application to thermosetting resins. **K. Kudo**, S. Fuse, M. Furutani, K. Arimitsu*

8:40 – 1054. From white board to product: Development of a nanocomposite material. **P. Beavis***

9:10 – 1055. Mechanical durability of interface controlled silica particulate composite. **K. SHINTANI**, C. Hongo, T. NISHINO

9:40 BREAK

9:55 – 1056. Toward rationally designed, additively manufactured carbon fiber composites with optimized mesostructures and orthotropic macroscale properties. **J.P. Lewicki***, E. duoss, W. Elmer, R.A. Fellini, M.J. King, M.L. Moffet, J. Rodriguez, T. Van Buuren, M.A. Worsley, A.S. Wu, C. Zhu

10:25 – 1057. Selective functionalization at photo-irradiated surfaces by using reaction development patterning. **T. Oyama***, K. Watanabe, H. Ogasawara

10:55 BREAK

11:00 – 1058. Designing the mechanical properties of additively manufactured silicone cellular solids with ordered microstructures. **T. Weisgraber**, J.P. Lewicki, A. Maiti, W. Small, S.C. Chinn, E. duoss, T.S. Wilson

11:30 – 1059. High molecular weight poly(*m,p*-phenylene)s derived by Suzuki polycondensation: Synthesis, processing, and testing. **B. Deffner***, D.A. Schlüter

Hawaii Convention Center
323A

New Perspectives of Bioplastics for Environmental Benign Materials (#396)

Organized by: U. Hiroshi, I. Chin,

T. Iwata, J. Li, P. Smith

Presiding: J. Li, P.B. Smith

8:00 – 1060. Novel polymeric materials from triglycerides. **H.N. Cheng***, A. Biswas

8:30 – 1061. Diacids and diols as renewable monomers for replacing oil-based harmful aromatics. **S. Kim***

9:00 – 1062. High performance and sustainable polyurethane materials by using new biobased aliphatic diisocyanate and its hardener. **T. Nakagawa**, H. Morita, S. Yamasaki

* Principle Author

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9:20 – 1063. Biobased sources for p-xylene. **P.B. Smith***, D.R. Henton, A. Dumitrescu, D.A. Hucul, M.N. Masuno, R. Smith, J. Bissell

9:40 – 1064. Highly heat-resistant polyesters from plant biomass-derived aromatic hydroxyl acids. **D. Ishii***, T. Iwata

10:00 – 1065. Potential al structural materials and chemo-enzymatic synthesis of poly(amine acid). **K. Numata***

10:30 – 1066. Development of biomass-based functional copolymers through grafting lignin via atom transfer radical polymerization. **J. Li***

11:00 – 1067. Controlled/living polymerization of styrenes derived from natural resources. **K. Sato***, M. Kamigaito

11:20 – 1068. Preparation of self-assembled chitin nanofiber-reinforced cellulosic materials. **J. Kadokawa***

11:40 – 1069. Chemoenzymatic synthesis of peptide capped with nylon4 unit at C-terminal aimed for thermally-processed peptide materials. **K. Yawaza***, K. Numata

Hawaii Convention Center
327

Advances in Precision Polymer Synthesis Using Reversible Deactivation Radical Polymerization (#401)

Organized by: D. Keddie, N. Tsarevsky, G. Moad, S. Yamago
Presiding: D. Keddie, N.V. Tsarevsky

8:00 – 1070. Controlled/living radical polymerization techniques in the synthesis of well-defined polymers containing reactive functional groups. **N.V. Tsarevsky**

8:30 – 1071. RAFT dispersion polymerization in nonpolar solvents. **S.P. Armes***

9:00 – 1072. Networks in the commercialisation of innovation projects using controlled radical polymerization (CRP).

D. Lusher*, M. Gilding, T. Spurling, G. Simpson, M. Flisher, I. Elsum, J. Brennecke, P. Wang, V. Bunton, T. Klein, B. Roden, J. Bralley

9:15 – 1073. Sustainable controlled/living radical polymerization with spinach extract. **S. Shanmugam***, J. Xu, C. Boyer

9:30 – 1074. Precision chemistry for the chain-end and mid-chain functionalisation of RAFT polymers. **S. Perrier***

10:00 – 1075. Industrial application of organotellurium-mediated living radical polymerization(ERP). **T. Shimizu**

10:30 – 1076. Polymer networks through tailored synthetic design. **T. Schiller***, D. Keddie

10:45 – 1077. End group removal of switchable RAFT agents. **S. Stace***, C. Fellows, G. Moad, D. Keddie

11:00 – 1078. Synthesis of single-ion BAB triblock nanostructured copolymers as efficient electrolytes for lithium metal batteries. **D. Gligme***

11:30 – 1079. Green polymer chemistry: Investigating the mechanism of radical ring-opening redox polymerization (R3P) of 3,6-diota-1,8-octanedithiol (DODT). **J.E. Puskas***, E.Q. Rosenthal-Kim

Hawaii Convention Center
323B

Aggregation Induced Emission: Materials and Applications (#444)

Organized by: M. Fujiki, B. Tang, B. Liu
Presiding: K. Ghiggino, D.T. Gryko, Y. Ma

8:00 – 1080. Biosensing/imaging with AIE fluorophores and polymorphism-dependent emission. **D. Zhang***

8:30 – 1081. AIE molecular crystal for organic light-emitting field-effect transistors. **Y. Ma***

9:00 – 1082. Excimers beyond pyrene: A far-red optical proximity reporter and its application based on aggregation-induced emission. **Y. Kim***

9:20 break

9:20 – 1083. Photoactivatable aggregation induced emission fluorophore-embedded silica nanoparticles functionalized with DNA aptamers. **A. Tong**, Y. Xiang, X. Wang, L. Peng

9:40 – 1084. Using aggregation induced emission to gain access to phosphorescent tellurophenes and benzotellurophenes. **E. Rivard**, G. He, W. Torres Delgado, D. Zomerman, B. Wilshire, K. Shankar, A. Brown

10:00 – 1085. AIE-lumigen-functionalized mesoporous materials: Fabrication and application. **J. Yu***

10:30 break

10:30 – 1086. New fluorescent probes for visualizing cell structures and function. **Y. Hong***

11:00 – 1087. Fluorescence color change in solid state due to the acrylonitrile derivatives polymorphs: Preparation, structures, and optical properties.

M.J. Percino*, M. Cerón, A. Bañuelos, G. Soriano-Moro, M. Castro, V. M. Chapelá, E. Pérez-Gutiérrez

11:20 – 1088. Restriction of intramolecular rotations via conjugation effect to efficiently enhance emission. **H. Nie, K. Hu, R. Hu, A. Qin***, **Z. Zhao***, B.Z. Tang*

11:40 – 1089. Aggregation-induced emission (AIE) effect of self-assembled diaztwist-pentacene microcrystals. **Q. Zhang**

Friday Afternoon

Hawaii Convention Center
324

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madsen, K. Saalwachter, Y. Yao, J. Battiste

Presiding: S. Kawahara, Y. Yao

13:00 – 1090. Elucidation of 3D nanoclusters of semicrystalline polymers embedded in single crystals by solid-state NMR.

T. Miyoshi*

13:25 – 1091. Probing the nanostructure, interphase, and dynamics of polymers and biopolymers by advanced multiscale solid-state NMR. **F. Wang**, R. Zhang,

P. Sun*, A. Shi

13:50 – 1092. Polymer functionalized nanoparticles and their nanocomposites: Solid-state NMR characterization.

L. Reven*, S. Allie, L. Zhu, H. Seo, V. Toader

14:15 – 1093. Polymers and interfaces in composite materials. **U. Scheier***

14:40 Break

14:55 – 1094. Structure and dynamics of polymers at the nanomaterials interface.

P.A. Mirau*, R. Naik

15:20 – 1095. Relaxation analyses of rubbers with carbon black and aging.

A. Asano*, M. Tsunomura, T. Ohkubo, K. Okushita, K. Numata, Y. Nakazawa

15:45 – 1096. Latex state NMR spectroscopy for rubbery polymers.

S. Kawahara*, S. Kewwarin

16:10 – 1097. Molecules, particles, and films: Dynamic NMR insights into polymer dispersions. **N. Nestle***

Hawaii Convention Center
325B

New Perspectives of Synthetic and Biological Soft Matter (#57)

Organized by: F. Horkay, J. Douglas, N. Choudhury, H. Jinna

Presiding: P. Bassar, N. Roy Choudhury

13:00 – 1098. Challenges for nanoscale imaging of soft materials by electron microscopy.

H. Jinna*, T. Higuchi

13:30 – 1099. Positron annihilation lifetime spectroscopy to probe molecular organization in self-assembled biomimetic systems.

A.J. Hill*, C. Fong, A.W. Dong, B.J. Boyd, C.J. Drummond

14:00 – 1100. Mechanical properties of well-defined polymeric hydrogels.

C.S. Patrickios*, E.J. Kepola, D.E. Apostolides, E.N. Kitiri, P.A. Panteli, T. Stylianopoulos, C. Voutouri

14:30 Break

14:40 – 1101. Longitudinal mapping of the mechanics of mouse knee articular cartilage.

E.K. Dimitriadis*, I. Morgan, E.L. Mertz, P.L. Chandran, F. Horkay

15:10 – 1102. Design and characterization of novel functional soft interfaces by polyelectrolyte brush immobilization.

A. Takahara*, Y. Higaki, M. Kobayashi

15:40 – 1103. β -Sheet nanocrystallite-reinforced synthetic thermoplastic elastomers.

L. Jia*

16:00 – 1104. Magic of interpenetrating networks based on ionic silicones and silicone elastomers.

S. Hvilsted*, L. Yu, A.L. Skov

16:20 – 1105. Influence of food additives on phase transition of thermosensitive polymer in aqueous solution.

H. Shimizu*, R. Wada, M. Okabe

16:40 – 1106. Impact of the ring density on the mechanical properties of polyrotaxane gels.

K. Kato, K. Ito

Hawaii Convention Center
323C

New Frontiers in Polymer Crystallization (#96)

Organized by: W. Hu, A. Toda, C. Li

Presiding: W. Hu, C. Li

13:00 Opening

13:05 Functional Materials

13:05 – 1107. Giant polyhedra and giant surfactants based on nano-atoms: Tuning from crystals, to quasicrystals, to Frank-Kasper phases.

M. Huang, K. Yue, W. Zhang, **S.Z. Cheng***

13:25 – 1108. Control over microphase separation, crystallization, and molecular orientation of all-conjugated diblock copolymers.

Y. Han

13:45 – 1109. Engineering crystal defects for enhanced ferroelectric properties in functional polymers.

L. Zhu

14:05 – 1110. Crystallization of protein-based composite materials.

X. Hu*

14:25 – 1111. Crystallization of biobased polymers with heterocyclic rings in the main chain.

H. Marubayashi*, T. Ushio, D. Aoki, S. Nojima

14:40 – 1112. Dissolution, hydrolysis and crystallization behavior of polyamide 6 in superheated water.

S. Yang*

14:55 Break

15:05 Molecular Simulations

15:05 – 1113. Role of the primitive path for crystallization and thickness selection in dense polymers.

J. Sommer, C. Luo

15:25 – 1114. Molecular simulation of crystallization in polymers: Beyond model linear polymers.

T. Yamamoto

15:45 – 1115. Conformation transitions of a polyelectrolyte chain in solution: A replica exchange Monte Carlo study.

P. Chi, L. Wang, **B. Li***

16:05 – 1116. Single molecule study of polymer interactions in single crystal: A combination of experiment and simulations.

W. Zhang, Y. Song, X. Lv, P. Yang

16:25 – 1117. Stepwise polymerization coupled with crystallization studied by molecular simulation.

Y. Ma*, J. Liu

Hawaii Convention Center
326A

Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158)

Organized by: T. Meyer, M. Ouchi, H. Steinman

Presiding: H. Steinman

13:00 – 1118. Precision structural control in sequence-defined peptoid polymers.

R. Zuckermann*

13:30 – 1119. Sequence-regulated Poly (ester-amide)s: Facile synthesis and properties.

Y. Wang, F. Du, **Z. Li***

14:00 – 1120. Biomimetic approaches to sequence controlled materials.

R.K. O'Reilly*

14:30 Break

14:40 – 1121. Sequence controlled polymers on DNA nanostructures.

H. Steinman*

15:10 – 1122. Making molecules with the tiniest machines.

D. Leigh*

15:40 – 1123. Syntheses of sequence-controlled polymers via consecutive multi-component reactions.

Z. Zhang*, J. Yan, **Y. You**

16:10 – 1124. Engineering polymer self-assembly via sidechain modification in phenylene vinylene polychromophores.

K.N. Plunkett

Hawaii Convention Center
325A

Macromolecular Self-Assembly for Smart Biomaterials (#196)

Organized by: S. Thayumanavan, L. Dai, J. Ryu
Presiding: S. Thayumanavan

13:00 – 1125. Macromolecular self-assembly as smart delivery systems for gene and oligonucleotide.

K. Kataoka*

13:25 – 1126. Importance of the intricate linkage of the needs of particular biomedical applications to the design characteristics of functionally-sophisticated nanoscopic macromolecules to achieve efficacy.

K. Wooley

13:50 – 1127. Polymers and nanoparticles for multiparameter immunoassays.

M. Winnik*

14:15 – 1128. siRNA delivery using polymers nanoparticles.

M. Monteiro

14:40 – 1129. Design of tunable multifunctional polymers for solubilizing highly lipophilic drugs.

T.M. Reineke*, J. Ting

15:05 Break

15:15 – 1130. Conjugated polymer nanoparticles for sensing, imaging, and therapy.

B. Liu

15:40 – 1131. Self-assembled organic nanoparticles for bioimaging and drug delivery.

Y. Zhao*

16:00 – 1132. Noncovalent polymer-gatekeeper in hollow nanoparticle for drug delivery platform.

J. Ryu*

16:20 – 1133. Multilocation-multistimuli-responsive degradation strategy for accelerated drug release.

J. Oh*

16:40 – 1134. Biomimetic polymersomes from controlled self-assembly of block copolymer.

S. Lecommandoux

Hawaii Convention Center
327

Cyclic and Topological Polymers (#248)

Organized by: Y. Tezuka, S. Grayson, M. Monteiro

Presiding: S. Grayson

13:00 Opening Remark

13:05 – 1135. Progress in the synthesis and characterization of cyclic polymers using the click cyclization approach.

S. Grayson

13:35 – 1136. Ring-closure methods for preparing cyclic polymers based on light-induced click chemistry.

K. Zhang*

*** Principle Author**

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14:05 – 1137. Evaluation of chain end coupling methods leading to macrocyclic vinyl polymers. **E. Tillman***
14:35 – 1138. Preparation of a cyclic macromonomer based on a cyclic thermo-responsive polyoxazoline and its copolymerization with water-soluble vinyl monomers. **M. Kubo***, M. Hioki, T. Uno, T. Itoh

14:55 Break

15:05 – 1139. Crystallization of cyclic PCL molecules and the effect of adding small quantities of linear PCL analogs. **A.J. Müller***, R. Perez, J.V. López, B. Zhang, S. Grayson
15:35 – 1140. Cyclic peptopeptides: Recent discoveries in the synthesis, characterization, and solution self-assembly. **D. Zhang**

16:05 – 1141. Thermoresponsive properties of linear- and cyclic-P(N-isopropylacrylamide) thin films. D. Magerl, M. Philipp, X. Qiu, P. Müller-Buschbaum, **F. Winnik**
16:25 – 1142. Synthesis and self-assembly of degradable cyclic graft copolymers. **A.P. Dove**, R.K. O'Reilly, R.J. Williams

Hawaii Convention Center
323A

Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294)

Organized by: T. Kato, M. Aizenberg, H. Kikuchi, S. Yu, H. Imai, C. Otsuki, C. Fraser, S. Kim

13:00 Opening Remarks

13:10 – 1143. Rationally designed microstructures. **J. Aizenberg***, W. Noorduin, A. Grinthal

13:40 – 1144. Photoresponsive self-assembled organic nanoparticles for bioimaging and drug delivery. **Y. Zhao***

14:10 – 1145. Janus polymer microparticles containing magnetic nanoparticles encapsulated in mussel-inspired amphiphilic polymers. H. Ohshima, Y. Saito, T. Higuchi, H. Yabu*

14:30 – 1146. Switchable dispersivity and molecular-trapping performance of mesostructured CaCO₃/thermosensitive polymer composite microspheres. **H. Imai**, A. Inoue, H. Tamagawa, Y. Oaki

14:50 Coffee Break
15:00 – 1147. Bioninspired fusion materials. **H. Cölfen***

15:30 – 1148. Supramolecular adhesion: Direct bond formation between organic and inorganic materials. **Y. Takashima**, A. Harada*

15:50 – 1149. Design of dynamic interface using hyperbranched polymers. **K. Tanaka***, R. Awane, M. Inutsuka, Y. Oda, H. Matsuno, N. Yamada, M. Haraguchi, M. Ozawa

16:10 – 1150. Self-assembly of mesogen-coated gold nanorods. **T. Hegmann***

16:30 – 1151. Interdisciplinary molecular self-assembly toward fusion materials. **N. Kimizuka**

Hawaii Convention Center
323B

Aggregation Induced Emission: Materials and Applications (#444)

Organized by: M. Fujiki, B. Tang, B. Liu
 Presiding: Z. Li, T.J. Müller, A. Qin

13:00 – 1152. Molecular recognition system orchestrated by self-assembly: From conventional AIE phenomena to assembly-based sensory systems. **T. Noguchi***, S. Shinkai

13:30 – 1153. Aggregation induced emission molecules: Design, synthesis, and stimuli response behaviors. **W. Tian***

14:00 – 1154. Fluorescent sensing for biomolecules via combining polyelectrolytes and AIE-active fluorophores. H. Xie, F. Zheng, Y. Wu, F. Zeng, **S. Wu***

14:20 break

14:30 – 1155. Complex of a DNA-switchable photosensitizer and triangular-shaped DNA origami for photodynamic therapy. X. Zhuang, Q. Jiang, C. Zhang, **G. Zou**, X. Liang

14:50 – 1156. Tuning luminescence of metal-organic frameworks for sensing applications. **B. Wang***

15:10 – 1157. Aggregation-induced emission (AIE) active polymers derived from tetraphenylethene and polyhedral oligomeric silsesquioxane (POSS) acrylates. **J. Xu**
 15:40 break

15:50 – 1158. Luminogenic polymers with aggregation-induced emission characteristics. **A. Qin***, B. Tang

16:20 – 1159. Organic luminescent materials: High efficient solid state emission and amplified spontaneous emission. **B. Xu***, S. Ma, J. Chen, W. Tian

16:40 – 1160. Supramolecular assembly induced emission enhancement in pillararene chemistry. N. Song, **Y. Yang**
17:10 – 1161. Discriminatively visualizing raft and non-raft domains in plasma membrane via a fluorescent probe with aggregation-induced red emission property. **J. Sun***, X. Yu

Friday Evening

Hawaii Convention Center
324

NMR Spectroscopy of Polymers and Biobased Materials (#12)

Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madsen, K. Saalwachter, Y. Yao, J. Battiste
 Presiding: L.A. Madsen

19:00 – 1162. Elucidating ion dynamics and structure in solid state organic conductors and ionic liquids using multinuclear NMR techniques. **M. Forsyth***, L. O'dell, K. Romanenko, L. Jin, H. Zhu, D. Gunzemann, J. Pringle

19:25 – 1163. Structure, dynamics and ionic conductivity of crystalline PEO/alkali-metal-salt complex polyelectrolytes – a solid-state NMR study. **Y. Yao***, L. Yang, X. Fu

19:50 – 1164. Behavior of water and proton in polymer electrolyte membrane: Insight into proton transfer mechanism. **O. Han***, J. Song, S. Han, S. Kim, H. Ha

Hawaii Convention Center
325B

New Perspectives of Synthetic and Biological Soft Matter (#57)

Organized by: F. Horkay, J. Douglas, N. Choudhury, H. Jinnai
 Presiding: E.K. Dimitriadis, J. Lisickiewicz

19:00 – 1165. Enzyme instructed supramolecular self-assembly in biological environment for biomedical applications. **Y. Gao***, F. Horkay

19:20 – 1166. Synergistic self-assembly of templating scaffolds with building blocks for directed synthesis of organic nanomaterials. **S. Dergunov***, A. Richter, M. Kim, S. Pingali, V. Urban, E. Pinkhassik

19:40 – 1167. Charge-separated peptide β -sheets: Sequence–secondary structure relationship for arranging charged side chains. **T. Nakayama***, T. Sakuraba, K. Tashiro, N. Ishii, Y. Yamamoto

20:00 – 1168. Naphthyl-based Val/Phe peptides as molecular sponges. **S. Martic***

20:20 – 1169. Unusual effect of topological structure of polymer chain on dynamic behaviour of polymer nanocomposites. **T. Tang***

20:40 – 1170. Morphological developments of diblock copolymers in thin film during solvent vapor annealing. **D. Lee***, T. Chang

Hawaii Convention Center
323C

New Frontiers in Polymer Crystallization (#96)

Organized by: W. Hu, A. Toda, C. Li
 Presiding: S.Z. Cheng, B. Lotz

19:00 Self-assembly of Block Copolymers

19:00 – 1171. Micelle engineering via living crystallization-driven block copolymer self-assembly. **G. Whittell***, I. Manners

19:20 – 1172. Regulation of the morphology of PCL-b-PEO crystalline micelles in aqueous solution by different methods. **J. Xu***, J. Yang

19:40 – 1173. Study on the physics of polymer crystallization based on the chain model of rod-coil multiblocks. **P. Tang**, J. Gao, H. Zhang, F. Qiu, Y. Yang

20:00 Surface- or Interface-induced

20:00 – 1174. Lamellar and molecular orientation of polyethylene and alkanes on graphene and related surfaces. R. Zhang, S. Park, **G. Unger**, X. Zeng, A. Tracz, O. Kwon, J. Jang

20:20 – 1175. Epitaxial crystallization of polymers: Structure control and mechanism. **S. Yan**

20:40 – 1176. Polymer crystallization at liquid-liquid interface. **C. Li***

Hawaii Convention Center
Halls I, II, III

Monomer Sequence Control: Using Nature's Strategy to Create 21st Century Polymers (#158)

Organized by: T. Meyer, M. Ouchi, H. Sleiman, Z. Li

Poster Session

19:00 – 21:00

1177. Control of iterative double monomer addition for sequence-controlled vinyl polymers. **K. Nishimori**, M. Ouchi*, M. Sawamoto*

Hawaii Convention Center
Halls I, II, III

Macromolecular Self-Assembly for Smart Biomaterials (#196)

Organized by: S. Thayumanavan, L. Dai, J. Ryu

Presiding: L. Dai

Poster Session

19:00 – 21:00

1178. Design of biodegradable nanosphere having cationic groups (II) - evaluation of DNA adsorption capacity. **K. Takahashi**, M. Fujita, Y. Takeoka, M. Rikukawa

1179. Poly-gamma-glutamic acid from *Bacillus licheniformis* CGMCC 2876 as a potential substitute for polyacrylamide in the sugarcane industry. **N. He***, S. Yan, L. Shen, Y. Peng

1180. Hydrogel lenses with surface-immobilized PEG layers for reduction of protein adsorption. **J.K. Lee**, H. Kim*

1181. Novel application of corn fiber gum in food processing: Emulsification, gelation, and starch behaviour modifying. **L. Yin**

1182. Host-Guest interaction mediated engineering of pH-responsive supramolecular vesicles for drug delivery. **B. Yang***, Z. Guo, L. Xiao, G. Zhou

1183. Introduction of flow photolithography and versatile applications. **J. Lee**

1184. Stimuli-responsive supramolecular assemblies of amphiphilic self-immovable polymers. **R.E. Yardley**, E.R. Gillies*, B. Fan, J.F. Trant, A.D. Wong, T.M. Gungor

1185. Multilayered micelles using PEG-P(Asp)-(PLLA) block copolymers for dual drug delivery. **K. Liu***, T. Fujiwara

1186. Synthesis of amphiphilic azobenzene molecules and their self-assembly, multi-stimuli-responsive properties. **Y. Xu***, M. R. Molla, B. Liu, K. R. Raghuvaran, L. Dai, S. Thayumanavan

1187. Coordination-responsive drug delivery systems based on selenium-tellurium-containing polymers. **W. Cao***, H. Xu

1188. Redox-responsive crosslinked nano-assemblies for drug controlled release. **C. Yuan**, L. Dai

1189. Self-healable polymer films from peptide-based multiblock polymers. **T. Koga***, T. Morishita, N. Higashi

1190. Controllable supramolecular polymerization through self-sorting of aliphatic and aromatic motifs. **L. Chen**, Z. Huang, J. Xu, X. Zhang

1191. Self-immolative polymersomes for high-efficiency triggered release and programmed enzymatic reactions. **G. Liu***, S. Liu

1192. Biodegradable amphiphilic polycarbonate bearing ratiometric fluorophores and H₂O₂-reactive pendent groups to serve as a multifunctional drug delivery platform. **C. Chen***, Y. Fu, C. Chen

1193. Porous biocompatible polymer nanocapsules with nanometer-thin walls: Synthetic approach and applications. **S. Dergunov***, M. Kim, E. Pinkhassik

1194. Synthesis and evaluation of PLLA diblock copolymer nanofiber (V)-effect of carboxyl group on nanofiber. **M. Kasatani**, M. Fujita, Y. Takeoka, M. Rikukawa

1195. Influence of the crosslinking degree and the inner structure on the nature of the gate effect in molecularly imprinted membrane. **K. Iwami**, Y. YOSHIMI*

1196. Spectroscopic study of the aggregation of cyanine dyes with different spacers in the presence of hyaluronic acid. **H. Tobata***, T. Sagawa

1197. Controllable supramolecular polymerization: The joint strategies of self-sorting and positive cooperativity. **Z. Huang**, X. Zhang

1198. Redox responsive coassemblies between selenium/tellurium-containing molecules and lipids. **L. Wang**, H. Xu

1199. Ferritin encapsulated Prussian blue nanoparticles for targeting photothermal therapy. **H. Chen**, G. FU, L. Zhao, Q. Qu, Y. Zhao

Hawaii Convention Center
Halls I, II, III

Cyclic and Topological Polymers (#248)

Organized by: Y. Tezuka, S. Grayson, M. Monteiro

Presiding: Y. Tezuka

Poster Session

19:00 – 21:00

1200. Preparation of cyclic polymer via ring-expansion NMP with two reactive sites. **T. Makino***, M.M. Matsushita, K. Awaga

1201. Ring-expansion living cationic polymerization: precision synthesis of ring-based functional polymers. **H. Kammiyada**, M. Ouchi*, M. Sawamoto*

1202. Precise construction of ring-based block copolymers. **T. Yamamoto**, M. Ouchi*, M. Sawamoto*, H. Kammiyada

1203. Modular construction of macrocycle-based topological polymers via high-efficient thiol chemistry. **J. Zhao***, J. Lu, N. Zhou, Z. Zhang, X. Zhu

1204. Versatile cyclic 2,2'-azobenzenophane with a functional handle and its polymers: Efficient synthesis and effect of topological structure on chiroptical properties. **J. Lu***, N. Zhou, Z. Zhang, X. Zhu

* Principle Author

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1205. Linear-cyclic polymer structural transformation using the dynamic property of rotaxane. **K. Nakazono***, T. Ogawa, S. Valentina, T. Takata*

1206. Block copolymer capable of undergoing linear-cyclic topology transformation using rotaxane protocol. **S. Valentina***, T. Ogawa, K. Nakazono, T. Takata

1207. Effective approach to cyclic polymer synthesis via transformation of macromolecular [1]rotaxane. T. Ogawa*, S. Valentina, K. Nakazono, T. Takata

1208. Construction and new applications of biomass-based cyclic poly lactones. Y. Zhu

1209. Synthesis of cyclic poly(tetrahydrofuran)s having axially chiral units and their thermally induced chiroptical responses. **S. Honda***, K. Adachi, T. Yamamoto, Y. Tezuka*

1210. Knotting probability of a cyclic DNA in solution through simulation. **E. Uehara**, T. Deguchi

1211. Separation and characterization of 4-arm star, 8-shaped, and tricyclic polystyrene. **J. Oh***, T. Chang

1212. Photo- and thermo-induced reversible transformation of cyclic and linear polymer topologies. **T. Yamamoto***, S. Yagyu, Y. Tezuka

1213. Topology effects by amphiphilic cyclic block copolymers on their vesicle and emulsion stabilization. **T. Yamamoto**, E. Baba, T. Yatsunuma, Y. Tezuka

1214. Giant micelle formation from cyclic poly(oxyethylene) alkyl ether surfactants. Y. Hirose

1215. Synthesis and characteristic properties of sun-shaped polymer having side chains of block copolymer. **T. Kono***, K. Adachi, Y. Tsukahara

1216. ESA-CF synthesis of cyclic and linear polymer having perylene diimide as pendant group and the investigation of electrical properties. **A. Kimura**, T. Yamamoto, Y. Tezuka

1217. Synthesis of phenolic resin with ladder shaped network. **H. Shoji**, T. Ogoshi, T. Yamagishi

1218. Star-shaped PHB-PLLA block copolymers generated through immortal polymerization with dinuclear indium catalysts. **T. Ebrahimi**, I. Yu, S.G. Hatzikiriakos, P. Mehrkhodavandi*

1219. Synthesis and characterization of a star polymer having changeable arm chain number. **T. Hirose***, D. Aoki, T. Takata

1220. Star/linear polymer topology transformation facilitated by mechanical linking of polymer chains. **D. Aoki***, S. Uchida, T. Takata

Hawaii Convention Center
Halls I, II, III

Advanced Membrane Separations (#262)

Organized by: R. Wickramasinghe, K. Tung, H. Chen, S. Husson
Presiding: H. Chen, S.M. Husson, K. Tung, R. Wickramasinghe

Poster Session
19:00 – 21:00

1221. Thermoplastic polymer functional nanofiber membranes prepared by melt blending extrusion: Application in Cr(VI) adsorption. **D. Xu**, R. Xiao

1222. Permeation of 2D polymer membranes (2): Improvement of oxygen permeability through polymer membranes by in situ reactions of functional groups of the 2D surface modifiers on the membrane surface. **J. Wang**, H. Urita, S. Takeo, M. Teraguchi, T. Kaneko, T. Aoki

1223. Tough ion gel membranes with organic-inorganic hybrid network for CO₂ capture. **E. Kamio**, T. Yasui, H. Matsuyama*

1224. Immobilization of poly(biphenylacetylene) derivatives bearing various polar groups onto silica gel and their application to chiral packing materials.

R. Ishidate, T. Sato, K. Shimomura, T. Ikai, K. Maeda, S. Kanoh, E. Yashima

1225. High performance thin-film composite FO membrane by using polyketone support. **M. Shibuya**, S. Mishima, m. yasukawa, T. Takahashi, T. Miyoshi, H. Matsuyama*

1226. Removal of viable bacteria and bacterial cytokine-inducing substances (CIS) by electro deionization (EDI) technology. T. Ase

1227. Transport properties of charge mosaic membranes prepared by polymer coating method. **Y. Kakihara**, N. Shigeta, A. Jikihara, M. Higa*

1228. Influence of electroosmotic flow on the ionic current rectification in a pH-regulated, conical nanopore. **S. Tseng***, D. Lin, J. Hsu

1229. Influence of concentration gradient on the ion transport in a pH-tunable poly-electrolyte brushes functionalized conical nanopore. **J. Lin**, J. Hsu*, S. Tseng

1230. Characterization of ion-exchange membranes prepared by ion irradiation graft polymerization method. **M. Goto**, T. Yamaki, H. Koshikawa, S. Sawada, A. Kitamura, M. Higa

1231. Power generation of reverse electrodialysis (RED) systems: The relationship between stack structure and performance of an RED system. **T. Sakurada***, M. Higa

1232. Ultrafiltration membrane-based osmotic heat engine with phase transition materials for enhanced power generation from low-grade heat. **T. Takahashi***, m. yasukawa*, A. Kumami, S. Osumi, H. Matsuyama*

1233. Evaluation of PRO power generation using forward osmosis membrane modules. **Y. Ikebe**, M. Higa

Hawaii Convention Center
Halls I, II, III

Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294)

Organized by: T. Kato, M. Aizenberg, H. Kikuchi, S. Yu, H. Imai, C. Otsuki, C. Fraser, K. Kim

Poster Session
19:00 – 21:00

1234. Mechanical properties of bulk films of deoxyribonucleic acid solid with chemical/physical cross-linking. **Y. Morimitsu**, H. Matsuno, K. Tanaka*

1235. Hierarchical porous polymers for a hydrophobic adsorbent derived from a biomaterial. **K. Sato**, Y. Oaki, H. Imai

1236. Synthesis and characterization of poly(vinyl acetate) derivative: A new candidate for blood compatible polymer. **K. Sato**, S. Kobayashi, H. Tagaya, M. Tanaka*

1237. Mechanistic study on anomalous photovoltaic effect in the ferroelectric liquid-crystalline phase of phenylterephthiophene derivatives. **A. Seki**, M. Funahashi*

1238. Formation of nonwoven fiber mats from collagen-like polypeptide. **S. Yoshida**, S. Morimune-Moriya, A. Sugawara-Narutaki, C. Ohtsuki*

1239. Structural color in the liquid crystalline nanosheet colloids of a layered clay and layered perovskites. S. Yamamoto, T. Sasaki, Y. Ebina, **N. Miyamoto***

1240. Adhesion of gels and glass substrates using covalent bond formation reactions. **T. Sekine**, Y. Takashima, A. Harada*

1241. Self-healing material able to change its color by various stimuli based on host-guest interaction between β -cyclodextrin and phenolphthalein. **K. Yonekura**, A. Harada*, Y. Takashima, M. Nakahata, H. Yamaguchi

1242. pH- and sugar-responsive gel assemblies based on boronate-catechol interactions. **S. Mori**, M. Nakahata, Y. Takashima, A. Harada*

1243. Adhesion between polymeric gels using various non-covalent interactions. **M. Nakahata**, Y. Takashima, A. Harada*

1244. Crystallization of phosphate in lyotropic liquid crystalline phases including simulated body fluid. **K. Nagaoaka**, H. Higuchi, Y. Okumura, C. Ohtsuki, T. Nishimura, T. Kato, H. Kikuchi*

1245. Creation of the nanostructure of π -conjugated polythiophene in the film. **K. Azuma***, T. Hayakawa, Y. Tanaka

1246. Preparation of monodispersed SiO₂-TiO₂ core-shell particles via the layer-by-layer assembly. **Y. Tanaka**, K. Katagiri, K. Inamura

1247. POSS-containing cylindrical polymer nanostructures for line patterning in block copolymer lithography. **F. Kato***, R. Maeda, S. Sugimoto, T. Hayakawa

1248. Self-organized chains of diblock copolymer micelles containing inorganic nanoparticles. S. Jang, K. Kim, J. Kim, B. Sohn*

1249. Synthesis of comb-like/block copolymer possessing polyethyleneimine brush and its application in silica deposition. **S. Eguchi**, R. Jin

1250. Preparation and application of chiral SiO₂ and Ag@SiO₂ materials using linear polyethyleneimine and tartaric acid. **S. Tsunega**, H. Murata, D. Yao, R. Jin

1251. Metal oxides formed on chiral silica frame. **m. sugimoto***, H. Murata, M. Saito, R. Jin

1252. Self-assembly behavior of crosslinked poly(sodium acrylate) microparticles based on molecular recognition. **T. Itami**, A. Hashidzume, H. Yamaguchi, A. Harada*

1253. Non-simple patterned nanocomposites through the block copolymer self-assembly. **S. Kim***, J. Lee, S. Choi, J. An

1254. Characterization of recombinant glasasin, a protein extracted from biosilica skeleton of the glass sponge Euplectella. **T. Amano**, J. Arima, K. Shimizu*

1255. Photochemical reactions on macroscopically organized multicomponent systems based on inorganic nanosheets. **T. Nakato***, E. Moura

1256. Preparation of supramolecular hydrogel composed of [c2]daisy chain. **K. Iwaso**, Y. Takashima, A. Harada*

1257. Addition of enzyme-like activity into simple β -sheet peptide and its application to bio-inspired calcium carbonate mineralization. **K. Murai***, T. Kinoshita, K. Nagata, M. Matsumoto, M. Higuchi

1258. Development and functionalization of liquid-crystalline complexes transporting ionic species. **T. Onuma**, J. Sakuda, E. Hosono, M. Yoshih, T. Ichikawa, T. Matsumoto, H. Ohno, H. Zhou, T. Kato*

1259. Anisotropic calcium carbonate nanocrystals formation using acidic macromolecules. **M. Nakayama**, S. Kajiyama, T. Nishimura, T. Kato*

1260. Luminescent fusion material of a sea urchin spine treated with europium complexes. **S. Ogata**, A. Ishii, Y. Oaki, H. Imai, M. Hasegawa

1261. Morphology control of inorganic crystal in thermotropic liquid crystalline phases. **T. Nakao**, H. Higuchi, T. Sajima, S. Daiki, Y. Okumura, T. Nishimura, T. Kato, H. Kikuchi*

1262. Preparation of protein-imprinted hydrogel layers fused with gold chips for surface plasmon resonance sensor and their responsive behavior. **Y. Kurio**, A. Kawamura, T. Miyata*

1263. Various thermoresponsive polymers with periodic carboxyl groups and higher-order structure in aqueous solution. **M. Uchiyama**, H. Sakaguchi, K. Satoh, M. Kamigaito*

1264. Region-specific accumulation of metal complexes at phase-segregation interface of normally oriented cylindrical nanostructure in amphiphilic liquid crystalline diblock copolymer film. **Y. Tanio**, M. Otonari, S. Asaka*, M. Noguchi, A. Izumi, H. Maeda

1265. Metal-organic framework tethering stimuli-responsive polymers for ON-OFF controlled release in solution. **K. Kokado***, S. Nagata, K. Sada*

Hawaii Convention Center
Halls I, II, III

Polymer Materials Performance, Degradation and Optimization (#369)

Organized by: M. Celina, T. Dargaville, H. Kudo, J. Lewicki

Presiding: M.C. Celina, H. Kudo, J.P. Lewicki

Poster Session

19:00 – 21:00

1266. Resist materials using base proliferation reactions. **T. Hashima**, K. Terada, M. Furutani, K. Arimitsu*

1267. Fabrication of positive-tone photopatterns by using photocyclization-type photobase generators. **S. Yoneda**, T. Ida, M. Furutani, K. Arimitsu

1268. Radiation resistance of electrical insulator for superconducting magnet system in high intensity accelerators. **A. Ideasaki***, T. Nakamoto, M. Yoshida, A. Shimada, M. Ito, K. Sasaki, M. Sugano, Y. Makida, T. Ogitsu

1269. Anionic UV curing of thick epoxy resin films by base amplifiers. **N. Shimoda**, Y. Koyama, M. Furutani, K. Arimitsu*

1270. Optimization of polymerization technique for reduction of micro pore volumes within synthetic resin adsorbents. **T. Kinoshita***, H. Fan, T. Kawakita, E. Furuya

1271. Study on storage condition of irradiated poly(etheretherketone) fabric for radiation-induced graft polymerization. **S. Saiki**, K. Okaya, H. Kudo*, N. Seko

1272. Preparation and hydrolysis of water-stable amorphous cellulose. **K. Hattori***, A. Arai

1273. Oxo-biodegradation of polystyrene under visible light irradiation. **K. Miyazaki**, H. Nakatani, T. Yoshida*

1274. Synthesis of and oxidative degradation of polystyrene-poly(diaicylhydrazine) block copolymer to obtain porous material. **M. Parvez**, N. Kihara*

1275. Preparation of optical resolution substance by the condensation of cyclodextrin and polysaccharides. **Y. Kitashima***, Y. Takada, S. Osawa

1276. Low-temperature film fabrication of colorless alicyclic polyimides with high T_g. **H. Ozawa**, E. Ishiguro, M. Suzuki, T. Matsumoto*

1277. Model reaction for alicyclic polyimide synthesis: Ring-opening reaction of asymmetric dianhydrides and chemical or thermal ring-closure of the amides. **M. Nagafuji**, H. Hattori, T. Matsumoto*

1278. Development of a *A. oryzae*/porous chitosan NF composite for degradation of formaldehyde. **A. Minemura***, R. Kitamura, M. Sano, S. Osawa

1279. Development of the biocompatible polymer with color functions by using natural pigments. **S. Onishi***, S. Shimasaki, S. Osawa

1280. Synthesis of inorganic poly(sulfonylhydrazine). **S. Horike**, N. Kihara*

1281. Radiation-induced reaction of fluorinated polymers and related compounds for extreme-ultraviolet lithography. **N. Nomura***, K. Okamoto, H. Yamamoto, T. Kozawa, R. Fujiyoshi, K. Umegaki

1282. Development of an antibiotic film material and its functional evaluation. **T. Sanada***, S. Osawa, O. Yoshimura, S. ODA

* Principle Author

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- 1283.** Pulse radiolysis study of resist polymers with and without photoacid generator. **K. Okamoto***, H. Yamamoto, T. Kozawa, R. Fujiyoshi, K. Umegaki
1284. Development and evaluation of novel polyimide/carbon fiber composite. **Y. Ishida***, T. Ogasawara, H. Kato, M. Miyauchi, N. Ooshiro, R. Yokota
1285. Measuring and analyzing the degradation of the epoxy resin under the high electric field by confocal Raman microprobe spectroscopy. **s. zhang***
1286. Photosensitive polyimide material containing photobase generator and fabrication of negative-tone micropatterns. **K. Okuyasu**, Y. Guo, T. Miwa, M. Furutani, K. Arimitsu*
1287. Soluble aromatic polyamides from unsymmetrical diamine containing two trifluoromethyl groups. **T. Byun***, S. Kim, I. Chung, S. Kim
1288. Ionic-liquid-assisted preparation of novel epoxy/MWNT nanocomposites with high radiation resistance. **J. Peng***, J. Li, M. Zhai
1289. Selective bond scission of phenolic polymers by oxidation with hypervalent iodine. **R. Kojima**, T. Ogoshi, T. Yamagishi
1290. Application to anionic UV curing of six-membered cyclic carbonate resins. **E. Nagai**, A. Sakauchi, M. Furutani, K. Arimitsu*
1291. Micro-photopatterning of trapped cycloolefin polymer via thiole-ene reactions. **A. Kakinuma**, I. Hazeyama, M. Furutani, K. Arimitsu*
1292. Evaluation of fractionized water-soluble chitosan for algicidal effect. **C. Choi**, H. Lee, S. Choi, G. Jeong, T. Kim, W. Kim, J. Nah*
1293. Inhibition effect of harmful algae using chitosan. **J. Nah***, T. Kim, G. Jeong, S. Choi, H. Lee, W. Kim, C. Choi
1294. Boron removal by glutamine chelate adsorbent grafted on polyethylene fabric. **N. Seko***, H. Amada, H. Hoshina
1295. Synthesis of fibrous adsorbent for dysprosium by radiation-induced graft polymerization. **H. Hoshina**, N. Seko*
1296. Long-term oxidation and free volume change of electron beam irradiated polymers. **T. Oka***, K. Onodera, Y. Kino, T. Sekine

Saturday Morning

- Hawaii Convention Center 324
NMR Spectroscopy of Polymers and Biobased Materials (#12)
Organized by: H. Cheng, A. English, H. Kaji, S. Kawahara, A. Whittaker, J. White, L. Madson, K. Saalwachter, Y. Yao, J. Battiste
Presiding: J.L. Battiste, A. English
8:00 – 1297. ^{19}F DOSY diffusion-NMR spectroscopy of fluoropolymers. **P.L. Rinaldi***, B. Ameduri, D. Chen, D. Fetherston, C. Gao, E. Kupce, X. Li*, G. Lopez, E. McCord*, E. Twum, Y. Wan, F. Wyzgorski, C. Xu
8:25 – 1298. Multidimensional NMR studies of perfluoropolyether. C. Xu, H. Yin, Y. Wan, X. Li*, P.L. Rinaldi
8:50 – 1299. Primary structural analysis of methacrylate copolymers by multivariate analysis of NMR spectra. **H. Momose***
9:15 – 1300. Analysis of chemical structures of synthetic polymers by solution NMR: SEC-NMR, DOSY, and multivariate analysis. **K. Ute***
9:40 Break
9:55 – 1301. New developments of LC-NMR for the characterization of polymers. **W. Hiller***, M. Hehn
10:20 – 1302. Application of cryoprobe technology to investigations of polymer degradation. **J.L. Battiste**
10:45 – 1303. Automation of quantitative NMR spectroscopy of polyolefins in industry. G. Hubner, L. Steiner, E. Pormakhina, **M. Parkinson***

- 11:10 – 1304.** ^{129}Xe NMR studies of biochar made from biobased materials. **H.N. Cheng***, M. Mauri*, R. Simonutti, M. Farina, G. Patriarca, T. Klasson
Hawaii Convention Center 326A

Radical Polymerization Kinetics and Process Modeling (#92)

- Organized by:* R. Hutchinson, G. Russell, P. Zetterlund, E. Saldivar-Guerra
8:00 Introductory remarks

- 8:05 – 1305.** Kinetics of radical polymerization in organic and aqueous solution studied via SP-PLP-EPR experiments. **H. Kattner***, **M. Babuck**

- 8:35 – 1306.** Influence of head-to-head addition on vinyl acetate propagation kinetics. **A.N. Nikitin**, O. Monyatis*, R. Hutchinson
8:55 – 1307. Kinetic studies of radical polymerizations based on direct observation of radicals by various ESR techniques. **A. Kajiwara***

- 9:15 – 1308.** Polymerization of acrylates: A world of surprise. N. Ballard, J. de la Cal, **J.M. Asua***
9:45 Break

- 10:00 – 1309.** Kinetics and modelling of atom transfer radical polymerization. **K. Matyjaszewski***

- 10:30 – 1310.** Limits of precision monomer placement in reversible deactivation radical polymerizations. **S. Harrisson***, S. Perrier, G. Gody, P. Zetterlund

- 11:00 – 1311.** Template radical polymerization in nanoreactors: A novel approach towards precision polymerization. A. Tardy, K. Bullar, S. Thickett, R. O'Reilly, **P. Zetterlund***

- 11:20 – 1312.** Engineering approach toward a universal RAFT system. A. Ilchev, L. Hlalele, R. Pfukwa, **B. Klumperman***

Hawaii Convention Center 323C

New Frontiers in Polymer Crystallization (#96)

- Organized by:* W. Hu, A. Toda, C. Li
Presiding: G. Ungar, Q. Xue

8:00 Thin Film and Confinement

- 8:00 – 1313.** Crystallization of polyesters in ultrathin films (blends, polycrystallomers and stereocomplexes). **R.E. Prud'homme***

- 8:20 – 1314.** Influence of crystallization temperature on melt-isothermal crystallization behaviors of poly(3-hydroxybutyrate) in thin films. **S. SASAKI***, J. Hoshiba, A. YASUDA, S. SAKURAI, H. Masunaga, T. Hikima, N. Ohta, M. Takata

- 8:40 – 1315.** Integrated ultrafast scanning calorimetric and micro-Raman spectroscopic investigation of polymer crystallization. **D. Zhou**

- 9:00 – 1316.** Morphological origins of double confined crystallization of PE-b-PS di-block copolymers within AAO nanoporous templates. **A.J. Müller***, M.T. Casas, R.M. Micheli, I. Blaszczyk-Lezak, J. Puiggalí, C. Mijangos, A.T. Lorenzo

- 9:20 – 1317.** Tuning the crystal orientation of PEO confined within AAO nanochannels. **H. Chen***

- 9:40 – 1318.** Confinement effects of nanoporous anodic alumina oxide on the crystallization of poly(vinylidene fluoride). **X. Sun**, S. Yan

9:55 Break

- 10:05** Rigid Chain and Copolymer

- 10:05 – 1319.** Crystalline helical monosubstituted polyacetylene: Molecular packing and shape actuation via phase transition. J. Wang, **E. Chen***

- 10:25 – 1320.** Crystallization behavior of poly(3-hexylthiophene). **Z. Su***

- 10:45 – 1321.** Melt structure and self-nucleation of ethylene copolymers.

- R.G. Alamo***, X. Chen, A. Mamun, M. Ren, Y. Sang

- 11:05 – 1322.** Nucleation of different crystalline forms in butene-1/ethylene random copolymer. **Y. Men***, Y. Wang, P. Liu, Y. Lu

- 11:25 – 1323.** Morphology and growth of propylene-ethylene random copolymer crystals in thin films. **K. Taguchi***, A. Fujikawa, A. Toda, T. Imai, K. Yamada

- 11:45 – 1324.** AFM imaging of semi-crystalline polymers with sub-molecular resolution. **N. Mullin***, R. Savage, J.K. Hobbs

Hawaii Convention Center 325B

Current Polyurethane Science (#133)

- Organized by:* K. Kojo, S. Hsu, K. Wynne, Z. Ren, S. Yamasaki, G. Zhang
Presiding: S. Yamasaki

8:00 Opening remarks

- 8:05 – 1325.** Ultra high-performance elastomers based on trans-1,4-bis(isocyanatomethyl cyclohexane). **S. Seneker***

- 9:05 – 1326.** Aliphatic poly(carbonate)glycols with different length of methylene unit and their polyurethane elastomers. **T. Masubuchi***, K. Kojo, M. Hurukawa

- 9:30 – 1327.** Synthesis and properties of polyurethanes crosslinked by polyrotaxanes. **N. Nonaka**, Y. Tanaka, H. Murakami

- 9:55 – 1328.** Highly efficient intramolecular hydroamination of polyallylurethane using macrocycle catalyst: Effect of polymer structure. **S. Mizuno***, D. Aoki, H. Sogawa, T. Takata

10:20 Break

- 10:35 – 1329.** Microbeam X-ray diffraction study on local anisotropic molecular aggregation structure of a thermoplastic polyurethane at the crack tip. **Y. Higaki**, K. Suzuki, N. Ohta, A. Takahara*

- 11:05 – 1330.** New biobased aliphatic diisocyanate and hardener using it, STA-BIOTM. **T. Nakagawa**, H. Morita, S. Yamasaki

Hawaii Convention Center 325A

Macromolecular Self-Assembly for Smart Biomaterials (#196)

- Organized by:* S. Thayumanavan, L. Dai, J. Ryu
Presiding: L. Dai

8:00 Thin Film and Confinement

- 8:00 – 1331.** Responsive polymer assemblies. **S. Thayumanavan***

- 8:25 – 1332.** Biomedical applications of di-block copolymer worm gels. **S.P. Armes***

- 8:50 – 1333.** Hierarchical assemblies of poly-produced amphiphiles for morphology-regulated cellular transport and intracellular triggered release. **S. Liu**

- 9:15 – 1334.** Conjugated polymer nanoparticles for in vivo molecular imaging. **J. Rao**

- 9:40 – 1335.** Stimuli-responsive polymer gels formed by host-guest interactions. **A. Harada***

10:05 Break

- 10:15 – 1336.** Many talents of polymeric networks: Methods for precise sizing of nano- and microscale structures with adaptive morphologies. **E. Harth***, B. Spears, K. Gilmore, D. Beezer

- 10:40 – 1337.** Supramolecular strategy for display of different functional groups at the inner and outer wall of synthetic vesicles and its impact on recognition of biomolecules. **S. Ghosh***

- 11:00 – 1338.** Tricontinuous (triple-network) morphologies in soft materials. **G.E. Schröder-Turk**, S.T. Hyde, M.G. Fischer, L. de Campo, J.J. Kirkensgaard

- 11:20 – 1339.** Functional yactowells for biological applications. **S.V. Bhosale***

- 11:40 – 1340.** Solution structure of branched peptides and polymer-peptide complexes in terms of the theories for branched polymers. **K. Terao**

Hawaii Convention Center 327
Cyclic and Topological Polymers (#248)

- Organized by:* Y. Tezuka, S. Grayson, M. Monteiro
Presiding: M. Monteiro

- 8:00 – 1341.** Various polystyrene topologies built from tailored cyclic polystyrene via CuAAC reactions. **M. Monteiro***

- 8:30 – 1342.** Synthesis of amphiphilic cyclic, figure-eight shaped, and tadpole-shaped block copolyethers. Y. Satoh, T. Isono, T. Kakuchi, **T. Satoh***

- 9:00 – 1343.** Modular constructions of topological and functional cyclic polymers. **Z. Zhang***, J. Zhao, J. Lu, N. Zhou, X. Zhu

- 9:30 – 1344.** Dynamics of cyclic polyethers by broadband dielectric spectroscopy. **F. Barroso-Bujans***, A. Alegra, J. Colmenero

9:50 Break

- 10:00 – 1345.** Zwitterionic ring-opening polymerization for the synthesis of cyclic polymers. **R. Waymouth***

- 10:30 – 1346.** Cyclic polymers from alkynes. C.D. Roland, H. Li, K.A. Abboud, K.B. Wagener, **A.S. Veige**

- 10:50 – 1347.** Macroyclic phenylenevinylene polymers: Synthesis and characterisation. **M.L. Turner***, B.J. Lidster, D. Kumar, Y. Tezuka, T. Yamamoto

- 11:20 – 1348.** Cyclic REMP polymers and other advanced materials from topological macromolecules. **G. Tew**

Hawaii Convention Center 323B

Advanced Membrane Separations (#262)

- Organized by:* R. Wickramasinghe, K. Tung, H. Chen, S. Husson
Presiding: S.M. Husson, R. Wickramasinghe

- 8:00 – 1349.** Reactive coating of filtration membranes with functional hydrogel layers for improved separation performance. **M. Ulbricht***, N. Alele, M. Birkner, M. Quilitzsch

- 8:20 – 1350.** Responsive membranes for advanced separations. **R. Wickramasinghe***, X. Qian

- 8:40 – 1351.** Thermoresponsive mesoporous block copolymer membranes with controllable response temperature. **Y. Tang***, H. Yokoyama, K. Ito, T. Ishizone

- 9:00 – 1352.** Stimuli-responsive DNA-apatamer gating membranes. **T. Schäfer***

- 9:20 – 1353.** Novel ultrafiltration membranes by reversible assembly of polymer brush nanoparticles. **I. Zharov**

- 9:40 – 1354.** Asymmetric self-assembled block copolymer membranes: Bridging the gap from ultra- to nanofiltration. **K. Peinemann***, H. Yu, x. Qiu, S. Nunes

- 10:00 – 1355.** Membrane morphology control and polymer solution rheology. **D.R. Wang***, W. Hung, S. Su

- 10:20 – 1356.** Surface patterning of polymeric membranes for fouling mitigation in separations of colloids, proteins, and ions. **Y. Ding**, S. Maruf, A. Greenberg, J. Pellegrino

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- 10:40 – 1357.** Membrane surface topology vs. surface chemistry for deposition resistance. **J. Pellegrino***, J. Mersch, X. Lu, S. Maruf, Y. Ding, A. Greenberg
- 11:00 – 1358.** Understanding the potential for nanopatterned surfaces to reduce membrane fouling. **M.S. Mauter**, S. Klara
- 11:20 – 1359.** Protein fouling detection on ultrafiltration membranes using ultrasonic reflectometry. **A.R. Lajmi***, E. Kujundzic, A. Greenberg, X. Wu
- 11:40 – 1360.** Polymer-brush coatings for membrane fouling resistance – toward theoretical design criteria. **G.Z. Ramon**

Hawaii Convention Center
323A

Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294)

- Organized by: T. Kato, M. Aizenberg, H. Kikuchi, S. Yu, H. Imai, C. Otsuki, C. Fraser, S. Kim
- 8:00 – 1361.** Luminescent boron beta-diketonate biomaterials for oxygen sensing and imaging. C.A. DeRosa, A. Mathew, J. Samonina-Kosicka, M. Kolpaczynska, Z. Fan, C.P. Kerr, J.N. Demas, H.C. Hendargo, D. Weitzel, C.L. Hofmann, G. Hanna, M.W. Dewhurst, G.M. Palmer, **C.L. Fraser**
- 8:20 – 1362.** Light-melt adhesive: Photomelting of flexible carbon frameworks in columnar liquid crystal phase. **S. Saito***
- 8:40 – 1363.** Polymers containing metal-ligands in their side chains: Coupling organic macromolecules to property rich inorganic metal ions. **G. Tew**
- 9:00** Coffee Break
- 9:10 – 1364.** Structure and function of metal organic frameworks in liquid/glass states. **S. Horike**
- 9:30 – 1365.** Circularly polarized luminescence of helical self-assembled lumophores with aggregation-induced emission characteristics. **B. Tang**
- 10:00 – 1366.** Fusion materials based on active poly(NIPAAm-co-AMPS) gels cross-linked by red-ox active Ru(II) complexes with new polymerizable bipyridine ligands: Synthesis, structure, and chemo-mechanical action in Belousov-Zhabotinsky reaction. **M. Aizenberg***, K. Okeyoshi, J. Aizenberg
- 10:20 – 1367.** Preparation of carbon-based fusion materials and their applications. **H. Nishihara***, T. Kyotani
- 10:50 – 1368.** Block copolymer lithography on chemically modified graphene. **S. Kim**
- 11:10 – 1369.** Fusion materials of lanthanide complexes with luminescence. **M. Hasegawa***
- 11:40 – 1370.** Coaxial nanowires having a carbon nanotube core and an inorganic shell. **Y. Takaguchi***, Y. Tango, K. Kurniawan, T. Tajima

Hawaii Convention Center
Halls I, II, III

Aggregation Induced Emission: Materials and Applications (#444)

- Organized by: M. Fujiki, B. Tang, B. Liu
- Poster Session**
10:00 – 12:00
- 1371.** Chiroptically enhanced luminescent π-conjugated polymer aggregates in controlled optofluidic medium. **M. Fujiki**
- 1372.** Design of a novel detection system through a combination of dynamic covalent bond formation and aggregation-induced emission. **D. Yoshihara**, S. Shinkai*
- 1373.** Specific light-up bioprobe with aggregation-induced emission and activatable photoactivity for targeted and image-guided photodynamic ablation of cancer cells. **B. Liu***, Y. Yuan, C. Zhang

- 1374.** Luminescent achiral polyfluorene meets chiral surface of cellulose triacetate during co-aggregation process. **S. Guo**, N. Abdul Rahim, N. Suzuki, M. Fujiki
- 1375.** Systematic fine-tuning of AIE and AIES in NPI (1,8-naphthalimide) based materials. **S. Mukherjee***, P. Thilagar*
- 1376.** Near-infrared selective AIE fluorogen for lipid droplet imaging in live cells. **M. Kang, Y. Zhao, X. Gu, C. Leung, J. W. Y. Lam, F. Li, B. Tang***
- 1377.** Novel fluorescent “turn-on” probe with aggregation-induced emission characteristic for cell apoptosis detection. **A. Leung, Y. Zhao, E. Zhao, J. W. Y. Lam, C. Leung, H. Deng, B. Tang***
- 1378.** Photostable AIE fluorogen for nucleolus and mitochondrion imaging with organelle-specific emission. **C. Yu*, Y. ZHANG, W. ZHANG, R. Kwok, B. Tang**
- 1379.** Ratiometric fluorescent probe for Hg^{2+} detection based on the alteration of the AIE behavior. **Y. Chen***, **Y. ZHANG**, J. W. Y. Lam, B. Tang
- 1380.** AIE-active turn-on bioprobe mediated by hydrogen bonding for highly sensitive detection of hydrogen peroxide and glucose. **Z. Song, H. Deng**, R. Kwok, J. W. Y. Lam, B. Tang*
- 1381.** A Dual-functional AEE fluorogen as a mitochondrion-specific bioprobe and an effective photosensitizer for photodynamic therapy. **E. Zhao, H. Deng**, J. W. Y. Lam, B. Tang*
- 1382.** Blue aggregation-induced emission lumogens: High external quantum efficiencies up to 3.99% in LED device, and restriction of the conjugation length through rational molecular design. **Z. Li**
- 1383.** Polyphenylbenzene as a platform for deep-blue OLEDs: Aggregation enhanced emission and high external quantum efficiency of 3.98%. **Z. Li**
- 1384.** Synthesis and characterization of a novel near-infrared bioprobe with aggregation-induced emission characteristics. **A. Nicol***, W. Qin, J. W. Y. Lam, B. Tang
- 1385.** Construction of efficient deep blue AIE lumogen from triphenylethene for non-doped OLED applications. **W. Qin**, **A. Nicol**, J. W. Y. Lam, B. Tang
- 1386.** Development of pure organic materials with long-lived and efficient room temperature phosphorescence. **W. Zhao**, **A. Nicol**, R.T. Kwok, J.W. Lam, B. Tang
- 1387.** Detection of oligomers and fibrils of α-synuclein by AIEgen with strong fluorescence. **C. Leung, Y. Hong, Z. Qiu**, J. W. Y. Lam, B. Tang*
- 1388.** Light-emitting polycyclic aromatic hydrocarbon synthesized by regioselective photocyclization and its application in optical waveguide. **X. Gu, Z. He, Z. Qiu**, J. W. Y. Lam, B. Tang*
- 1389.** Development of functional poly(triphenylacrylonitrile) with in situ generated AIEgen by three-component polymerization of aryl bromides, internal alkynes, and potassium ferrocyanide. **Z. Qiu**, J. W. Y. Lam, B. Tang*
- 1390.** Construction of conjugated fluorescent polymers through transition-metal-free homopolymerization of difunctional haloalkynes. **Y. ZHANG***, J. W. Y. Lam, B. Tang
- 1391.** Optical properties of solid-emissive BODIPYs bearing aryl substituents at the boron center. **H. Yamane**, S. Ito, K. Tanaka*, Y. Chujo*
- 1392.** Stable AIE lumogen carrying acyl chloride functionality as fluorescent visualizer for intracellular imaging. **Z. Wang**, E. Zhao, Z. Zhao, B. Tang*
- 1393.** Synthesis and properties of pyrrole derivatives emitted red fluorescence with aggregation-enhanced emission feature. **G. Liu, J. Shi***, B. Tong, Y. Dong
- 1394.** Bifunctional AIE lumogen as selective mitochondrial-targeting probe for cancer cell and photosensitizer for photodynamic therapy. **C. Gui, E. Zhao**, **Z. Wang**, J. W. Y. Lam, B. Tang*
- 1395.** Selective staining of mitochondria by a non-leaking tetraphenylethene-based dye with red emission. **J. Roose**, **W. ZHANG**, **Z. Wang**, J. W. Y. Lam, B. Tang*
- 1396.** Transferrin-functionalized nanoparticles with aggregation-induced emission characteristics for image-guided and targeted photodynamic cancer therapy. **X. Cai, S. Xu, B. Liu***
- 1397.** Ultrabright organic dots with aggregation-induced emission characteristics for cell tracking. **G. FENG, X. Cai, B. Liu***
- 1398.** Platinum prodrug conjugated with photosensitizer with aggregation-induced emission (AIE) characteristics for drug activation monitoring and combinatorial photodynamic–chemotherapy against cisplatin resistant cancer cells. **Y. Yuan**, **X. Cai**, **B. Liu***
- 1399.** Self-assembly-induced fluorescence turn-on for specific protein imaging. **H. Wang, D. Ding**
- 1400.** Self-assembly of a light-up AIE probe in targeted cancer cells for long-term fluorescent cell tracking. **D. Ding**, **G. Wang**
- 1401.** Photoexcited chirality transferability from chiral biphenyl to achiral anthracene revealed by circularly polarized luminescence study. **S. Kitamura**, K. Nakabayashi, N. Tajima, T. Harada, M. Fujiki, **Y. Imai**
- 1402.** Nano graphene oxide modified aggregation-induced emission nanoparticle and Its application in *in vivo* bioimaging. **Z. Zhu***, W. Qin, D. Li, J. Qian*
- 1403.** Efficient AIE-active pure blue molecule by incorporating multifunctional groups into tetraphenylsilane. **P. Lu***, X. Tang
- 1404.** Real-time fluorescent chemosensor based on aggregation-enhanced emission for quantitative monitoring trace carbon dioxide gas. **H. Wang**, **P. Liu**, D. Chen, Y. Zhang, J. Shi, X. Feng, B. Tong, **Y. Dong***
- 1405.** Preparation of optical-active polysiloxanes with aggregation-induced emission property. **L. Dong**, N. Jin, K. Liang, J. Zhi*, B. Tong, **Y. Dong***
- 1406.** Aggregation-induced emission properties and self-assembly of aryl-substituted 1,2,5-triphenylpyrrole derivatives. **N. Jin**, Y. Zhang, J. Shi, J. Zhi*, B. Tong, **Y. Dong***
- 1407.** Fluorescent sensing for hyaluronidase via combination of AIE and ACQ effects. **H. Xie***, F. Zeng, **S. Wu**
- 1408.** Fluorescent sensing for alkaline phosphatase via excimer/monomer conversion. **F. Zheng**, F. Zeng, **S. Wu**
- 1409.** Probing sugar-lectin recognitions based on glyco-diketopyrrolopyrrole with aggregation-induced NIR emission. **Y. Hang**, **J. Hua**
- 1410.** Diketopyrrolopyrrole-based NIR fluorescent biosensor for BSA detection and AIE-assisted bioimaging. **Y. Hang**, **J. Hua**
- 1411.** Design and synthesis of new tetraphenylpyrazine-based AIEgens. **A. Qin***, B. Tang
- 1412.** Aggregation-induced emission of hexaphenyl-1,3-butadiene. **Y. Zhang**, L. Kong, J. Shi, B. Tong, Y. Dong*
- 1413.** Novel conjugative hyperbranched polymers with aggregation-induced emission characteristics: Synthesis by one-pot “A2 + B4” polymerization, application as explosive chemosensors and PLEDs. **X. Chen**
- 1414.** Conjugated hyperbranched polymer constructed from carbazole and tetraphenylethylene moieties: Convenient synthesis through one-pot “A2 + B4” Suzuki polymerization, aggregation-induced enhanced emission, and application as explosive chemosensors and PLEDs. **X. Chen**
- 1415.** Graphene oxide-based AIE biosensor with high selectivity toward bovine serum albumin. **X. Chen**
- 1416.** Reversible near-infrared/blue mechanofluorochromism of aminobenzopyran-oxanthene. **M. Tanioka**, S. Kamino*, A. Muranaka*, Y. Ooyama, H. Ota, Y. Shirasaki, J. Horigome, M. Ueda, M. Uchiyama, D. Sawada, S. Enomoto
- 1417.** Charge transfer properties-molecular structure of α,β -unsaturated acrylonitrile compounds experimental and computational chemistry point of view. **M.J. Percino**, M. Cerón, O. Rodriguez Meza, M. Castro, G. Soriano-Moro, V. M. Chapela, E. Pérez-Gutiérrez, J. Ricardo
- 1418.** Fabrication and stimuli-triggered disintegration of crosslinked gel networks with switchable fluorescence emissions. **J. Hu**, **S. Liu***
- 1419.** Micellar nanoparticles with pH-tunable micellization mechanism and aggregation-induced emission. **S. Tian**, **Y. Li**, **S. Liu***
- 1420.** Amphiphilic star copolymers for bacteria detection and elimination. **Y. Li**, **S. Liu***
- 1421.** Proton-triggered hypsochromic luminescence in 1,1'-(2,5-distyryl-1,4-phenylene) dipiperidine. **J. Chen**, **B. Xu**, **W. Tian***
- 1422.** Reversible multistimuli-response fluorescent switch based on tetraphenylethene-spiropyran molecules. **Q. Qi**, **B. Xu**, **W. Tian***
- 1423.** Selective tumor cell imaging using DNA aptamer-functionalized AIE fluorophore-embedded silica nanoparticles. **A. Tong***
- 1424.** Turn-on sensing for Ag⁺ based on AIE-active fluorescent probe and cytosine-rich DNA. **K. Ma**, **H. Wang**, **B. Xu**, **W. Tian***
- 1425.** Highly efficient near-infrared organic dots based on novel AIE fluorogen for specific cancer cell imaging. **Y. Zhang**, **B. Xu**, **W. Tian***
- 1426.** Fluorescence behavior of single polyfluorene nanoparticles. **S. MACHIDA***, Y. Hashimoto, N. Ikeda
- 1427.** Synthesis of silole-peptide dendrimer for targeting norovirus-3C protease. **B.D. Sandanala**, T. Furukawa, T. KOYAMA, K. MATSUOKA, K. Hatano*
- 1428.** Amphiphilic dipolar π-conjugated systems with smart luminescence properties. **Y. Hirai**, S. Yagai
- 1429.** Development of diagnosis tools for Alzheimer's diseases based on AIE phenomenon. **T. Murashima***, K. Kawamura, R. Nakayama, A. Matsumoto, S. Fujii*
- 1430.** Imidazole-appended p-phenylene-Cu(II) ensemble as a chemoprobe for histidine in biological samples. **K. Kim**, J. Jung*
- 1431.** Preparation and characterization of aniline dimer derivative with aggregation-enhanced emission properties. **H. Lu**, K. Wang, **J. Yang***
- 1432.** Tuning the luminescence of metal–organic frameworks for detection of energetic heterocyclic compounds. **L. Wang**, X. Feng, B. Wang*
- 1433.** Multiphoton absorption property of a single crystal of luminescent gold complex. **A. Ando**, S. Yamada, O. Tsutsumi*, K. Kamada
- 1434.** Mechanofluorochromic polyurethanes with aggregation-enhanced emission feature. **K. Wang**, H. Lu, J. Yang*
- 1435.** Syntheses of AIE dye labeled biomolecular probes aiming to the development of facile diagnosis methods for cancer and Alzheimer's disease. **K. Kawamura***, A. Matsumoto, T. Murashima

* Principle Author

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- 1436.** Tuning of luminescent color from a gold complex without modification of molecular structure. **R. Kawano**, S. Yamada, O. Tsutsumi*
- 1437.** Crystallization-induced phosphorescence of Pd(Ph₃)₄. **M. Gao**, A. Qin*, B.Z. Tang*
- 1438.** Multiscale simulation on excited state dynamics in amorphous organic aggregates. **H. Ma**, Q. Peng*, Z. Shuai*
- 1439.** Construction of nanoparticles using TICT type BODIPYs. **A. Matsumoto***, K. Kawamura, T. Murashita
- 1440.** Tetraphenylethene-based derivatives for supramolecular self-assembly. **A.S. Ranawade**, S.V. Bhosale
- 1441.** Circular supramolecular polymers: A mechanistic study. **K. Aratsu**, S. Yagai
- 1442.** Synthesis of fluorescence detection against pathogens based on the aggregation-induced emission effect. **K. Nakamura**, T. Furukawa, T. KOYAMA, K. Hatano
- 1443.** Synthesis of fluorescence silole-core dendrimers carrying sugar chain as pathogen sensor. **S. Matsumura***, K. Nakamura, T. Furukawa, T. KOYAMA, K. MATSUOKA, K. Hatano
- 1444.** Tetraethoxyethylene TTE and tetrafluoroethylene TFE: New promising AIE luminogens. **L. Viglianti***, N. Xie, A. Bolzoni, C. Baldoli, P. Mussini, R. Kwok, J. W.Y. Lam, E. Licandro*, B. Tang*
- 1445.** White-color emitting polymer materials containing liquid-crystalline gold complexes. **O. Tsutsumi***, O. Younis, S. Tamai, S. Yamada
- 1446.** Perfluoroalkyl-substituted rod-shaped gold(l) complexes as new solid-state luminescent materials. **S. Yamada**, O. Tsutsumi*
- 1447.** Traceable drug delivery system for next generation drugs based on aggregation-induced emission compounds and fluorescent proteins. **M. Suzuki**, K. Hatano
- 1448.** Highly fluorescent metal-organic frameworks constructed from molecules with aggregation-induced emission properties. **Y. Zhang**, Y. Guo, X. Feng, B. Wang*
- 1449.** Electrochemistry of heterocycle-based ethenes: Molecules displaying aggregation-induced emission features. **L. Viglianti***, A. Bolzoni, C. Baldoli, E. Licandro*, P. Mussini*
- 1450.** Synthesis and optical properties of aggregation induced emission dyes based on maleimide skeleton. **H. Imoto**, K. Kizaki, K. Naka*
- 1451.** Synthesis, structure, and solid-state photophorescence of *trans*-bis(salicylaldiminato)platinum(II) complexes bearing perpendicular aromatic units with intramolecular Pt-H interactions. **S. Iwata**, H. Takahashi, N. Komiya, T. Naota*
- 1452.** 3,14-Diaryl-17,17-diphenyltetrabenzofluorenes: New fluorophores displaying both aggregation-induced emission and remarkable solvatochromism. **T. Kawase***
- 1453.** Photofunctional dendrimers based on the AIE/AIEE luminogens: Light-harvesting and sensing. **Y. Li***, Y. Zeng*
- 1454.** Aggregation induced simultaneous enhancement of luminescent efficiency and charge mobility in fluorene-based copolymer. **L. Liu**, Y. Ma*
- 1455.** Enhanced solid-state ESIFT luminescence of imidazopyridine derivatives: Polymorph dependence and stimuli-responsive behavior. **T. Mutai***, Y. Shigemitsu, H. Shono, T. Ohkawa, H. Sawatani, K. Araki*
- 1456.** Highly selective fluorogenic multianalyte biosensors constructed via enzyme-catalyzed coupling and aggregation-induced emission. **X. Wang**, S. Liu
- 1457.** H₂O₂ and pH-responsive organogel with aggregation-induced emission and chemiluminescence constructed via thiolene click reaction. **X. Wang**, J. Hu, S. Liu
- 1458.** Luminescent liquids crystals: Aggregation-induced emission and phase behaviors. **Z. Yu***, M. Li, J. Li, W. Li, J. W.Y. Lam, B. Tang

- 1459.** Series of abnormal tetrahydropyrimidine-based AIE compounds: Application and AIE origin. **Q. Zhu**
- 1460.** Through-space conjugated folded tetraphenylethene derivatives with high fluorescence efficiencies and remarkably large Stokes shifts. **B. He**, H. Nie, R. Hu, A. Qin, Z. Zhao*, B.Z. Tang*
- 1461.** Steric and conjugation effects on the aggregation-induced emission of phosphindole oxide fluorophores. **F. Bu**, R. Hu, A. Qin, Z. Zhao*, B.Z. Tang*

Saturday Afternoon

Hawaii Convention Center
324

Dynamic, Reversible, and Self-healing Materials (#64)

Organized by: W. Skene, H. Otsuka, S. Rowan
Presiding: S.J. Rowan, W. Skene

13:00 – 1462. Adaptable and stimuli-responsive polymer networks. **C.N. Bowman***, G. Berg, M. McBride, N. Sowan, S. Chatani, M. Podgórski

13:30 – 1463. Compact polyelectrolyte complexes: New materials with astonishing mechanical and self-healing properties. **P. SCHAAF***, J. Schlenoff

13:45 – 1464. Reversible morphological transformation through dynamic covalent self-assembly. **K. Baek**, K. Kim*

14:00 – 1465. Adhesive materials utilizing molecular interaction of thymine-adenine and photodimerization of thymine. **N. Ishikawa***, M. Furutani, K. Arimitsu

14:15 – 1466. Ionically crosslinked polymer networks. **K. Cavicchi**, G. Deng, J. Lee

14:30 coffee

14:45 – 1467. Multiphase design of dynamic self-healing polymer design via both noncovalent and dynamic covalent interactions. **Z.M. Guan***

15:15 – 1468. Self-healable adhesion system by immobilized polyelectrolyte brush. **A. Takahara**, M. Kobayashi

15:30 – 1469. Preparation of novel self-healing unsaturated polyester resin. **Y. Kajihara**, J. Nunoshige, T. Muraki

15:45 – 1470. Freezing-induced mechanochemistry using dynamic covalent mechanophores. **K. Imato**, A. Takahara*, H. Otsuka*

16:00 – 1471. Development and testing of intricate, amphiphilic crosslinked hyper-branched fluoropolymers as anti-icing coatings in aerospace and defense applications. **J. Summerhill**, K.A. Pollack, J.E. Raymond, K. Wooley*

16:15 – 1472. New metal-free azide-alkyne click reaction for self-healing polymer films. **S. Fukushima**, T. Michinobu

16:30 – 1473. Control of structure and chirality in dynamic and reversible supramolecular polymers. **M. Raynal***, A. Desmarchelier, V. Ayzac, P. Brocorens, N. Vanthuyne, L. Bouteiller

Hawaii Convention Center
326A

Radical Polymerization Kinetics and Process Modeling (#92)

Organized by: R. Hutchinson, G. Russell, P. Zetterlund, E. Saldivar-Guerra

13:00 Introductory remarks

13:05 – 1474. Strength of model-based design for the synthesis of well-defined macromolecular architectures via a radical mechanism. **D.R. D'hooge***, P. Van Steenberghe, M. Reyniers, G. Marin

13:35 – 1475. Push monomer conversion high and understand diffusion-controlled reactions in CRP. **S. Zhu***

14:05 – 1476. Determination of copolymerization reactivity ratios on vapor-phase assisted surface copolymerization (VASP) by nonlinear least-squares method. **S. Iwakiri***, H. Nishida

14:25 – 1477. Autoacceleration in the free-radical polymerization of methyl methacrylate and vinyl acetate: A comparative study. **D. Victoria-Valenzuela**, J. Herrera-Ordonez*

14:45 Break

15:00 – 1478. Overview of Monte Carlo methods in polymer reaction engineering. **J.B. Soares***

15:30 – 1479. Modeling of VDF/HFP copolymerizations considering transfer to polymer reactions and secondary radical propagation. **S. Beuermann***

16:00 – 1480. Analytical solution of free radical polymerization: Application to the numerical modeling and simulation of polymerization reactions in coiled flow inverters. **D.K. Garg**, C.A. Serra*, D. Parida, Y. Hoarau

16:20 – 1481. Simulation of radical polymerization of methyl methacrylate at room temperature using a tertiary amine/BPO initiating system. **A. Zoller**, D. Gigmes, Y. Guillaneur*

Hawaii Convention Center
323C

New Frontiers in Polymer Crystallization (#96)

Organized by: W. Hu, A. Toda, C. Li
Presiding: M. Hikosaka, G. Strobl

13:00 Kinetics

13:00 – 1482. Melting kinetics of polymer crystals. **A. Toda***, T. Ando, K. Taguchi, K. Nozaki, M. Maruyama, Y. Mizutani, K. Tagashira, T. Fukushima, H. Kaji, K. Monishi

13:20 – 1483. Influence of entanglements on melting behavior of a semi-crystalline polymer. **S. Rastogi***, S. Ronca, D. Romano, G. Forte, K. Liu, E. Andabalo-Reyes

13:40 – 1484. Role of temperature, chain length, and crystal structure in the mechanism of quiescent polymer crystal growth by chain-folding. **H. Marand***

14:00 – 1485. Elucidations of chain folding and unfolding of semicrystalline polymers by solid-state NMR. **T. Miyoshi**

14:20 – 1486. Formation and 3D-structure of shish-kebab in semi-dilute solution of ultrahigh molecular weight polyethylene. **H. Murase***, T. Hashimoto*

14:40 – 1487. Crystal nucleation and growth kinetics in polymers, studied by Tammann's development method and fast scanning calorimetry. **E. Zhuravlev***, J.W. Schmelzer, A.S. Abzyov, V.M. Fokin, R. Androsch, C. Schick

14:55 Break

15:05 Morphology and Mesomorphic Phase

15:05 – 1488. Effect of the crystalline α -process on the morphology of semicrystalline polymers: A comparative SAXS/NMR-study on poly(ϵ -caprolactone) and polyethyleneoxide. **A. Seidlitz**, R. Bärenwald, K. Saalwaechter, **T. Thurn-Albrecht***

15:25 – 1489. Controlled handedness of twisted lamellae in banded spherulites of chiral polymers. **R. Ho**

15:45 – 1490. Temperature reversible structure change of semi-crystalline polymers studied with temperature modulated X-ray scattering. **Y. Saruyama***

16:05 – 1491. Vitrification, mesophase formation, and crystallization of poly(butylene-2,6-naphthalate). **K. Nishida***, E. Zhuravlev, B. Yang, C. Schick, T. Kanaya

16:25 – 1492. Some aspects of nucleation in polymorphic isotactic poly(1-butene). **D. Cavallo**, L. Gardella, G.C. Alfonso

16:45 – 1493. Interpretation of temperature dependences of spherical growth rate and lamellar thickness by polymer crystallization model through the mesophase. **T. Konishi***, D. Tadokoro, W. Sakatsui, K. Fukao, Y. Miyamoto

Hawaii Convention Center
325B

Current Polyurethane Science (#133)

Organized by: K. Kojo, S. Hsu, K. Wynne, Z. Ren, S. Yamasaki, G. Zhang
Presiding: K. Kojo

13:00 – 1494. Novel polyhydroxyurethane thermoplastic elastomers: Critical role of the hydroxyl group and the chemical structure of the soft segment in controlling nanophase separation required for elastomeric behavior. **E. Leitsch**, K. Liu, K. Scheidt, **J. Torkelson***

14:00 – 1495. Thermoplastic polyhydroxyurethane as non-isocyanate polyurethane elastomer. **G. Beniah**, K. Liu, N. Wilmot, W.H. Heath, K. Scheidt, J. Torkelson

14:30 – 1496. RZETA – new amine catalyst for polyurethane with low amine emission. **Y. Sesoko**, H. Fujiwara, T. Suzuki, H. Kiso, J. Tucker

15:00 Break

15:15 – 1497. Liquid-crystalline behavior of binary systems consisting of polyurethane mesogens and polar nematic liquid crystals. **Y. Shima**, M. Nata, S. Ujiiie*

15:40 – 1498. Thermotropic liquid-crystalline polyurethanes and their metal-complexed family. **S. Ujiiie***, Y. Shima, G. Shimada, M. Nata

16:10 – 1499. Polyurethane-peptide hybrids: Hierarchy and mechanics inspired by nature. **L. Korley***, J. Johnson, L. Matolay, N. Wanasekara

16:35 – 1500. High-efficient CO₂-based polyurethane hot melt adhesives. **Z. You**, Z. Liu, J. Chu

Hawaii Convention Center
325A

Macromolecular Self-Assembly for Smart Biomaterials (#196)

Organized by: S. Thayumanavan, L. Dai, J. Ryu
Presiding: J. Ryu

13:00 – 1501. Virus nanoreactors and the hierarchical assembly of coupled catalytic materials. **T. Douglas***

13:25 – 1502. Modular assembly of diagnostic nanoparticles and therapeutic stem cells. **H. Kong**

13:50 – 1503. Design and self-assembly of a polymer prodrug for tissue regeneration. **J. Cheng**, P. Messersmith*

14:15 – 1504. Smart polymers for protein conjugates, protein nanoparticles and reversible nanopatterning. **H. Maynard**, M. Lorenzo, E. Lin, N. Matsumoto, E. Bat

14:40 – 1505. Adaptive peptide nanostructures through (non-) equilibrium biocatalytic self-assembly. **R.V. Ulijn***

15:05 Break

15:15 – 1506. Enzyme-instructed self-assembly (EISA) for cancer therapy. **B. Xu**

15:40 – 1507. In situ cross-linking and stimuli-responsive degradation of macromolecular multilayers for cell encapsulation. **S. Yang***, I. Choi, J. Ryu

16:00 – 1508. Self-assembled dendron-polymer conjugates as drug delivery vehicles. **R. Sanyal***

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16:20 – 1509. Light-triggered drug delivery systems using a dendrimer-gold nanorod composite membrane. **M. Park***

16:40 – 1510. Trading of DNA oligomers encapsulated into self-assembled microsphere. **N. Morimoto***, R. Takei, S.M. Nomura, M. Suzuki

Hawaii Convention Center
323A

Cyclic and Topological Polymers (#248)

Organized by: Y. Tezuka, S. Grayson, M. Monteiro
Presiding: Y. Tezuka

13:00 – 1511. Catenated and knotty living polymerizations. **R. Advincola***

13:30 – 1512. Reversible topology transformation of linear - cyclic polymer using rotaxane protocol. **T. Takata***

14:00 – 1513. Flexibility, nesting, and stacking in cyclic porphyrin polymers. L. Perdigao, A. Esmail, A. Summerfield, S. Svatek, D. Kondratuk, A. Stannard, H. Anderson, P. Beton*

14:20 – 1514. Application of graph theory and knot theory to polymer chemistry. **K. Shimokawa**

14:50 Break

15:00 – 1515. Racemic and quasi-racemic X-ray structures of cyclic disulfide-rich peptide drug scaffolds: Looking into the mirror for drug design. **D. Craik**, C. Wang, G. King, S. Northfield, P. Ojeda

15:30 – 1516. Using the cyclotide scaffold to target protein-protein interactions. **J.A. Camarero***

16:00 – 1517. Folding single polymer chains into defined geometries. **C. Barner-Kowollik***

16:30 – 1518. Topological polymer chemistry designing macromolecular graph geometries. **Y. Tezuka***

Hawaii Convention Center
323B

Advanced Membrane Separations (#262)

Organized by: R. Wickramasinghe, K. Tung, H. Chen, S. Husson
Presiding: K. Tung

13:00 – 1519. Tunable multifunctional membranes for water treatment to enzyme catalysis: An overview. **D. Bhattacharya***

13:20 – 1520. Development of novel osmotic membranes for water and energy applications. **R. Wang***

13:40 – 1521. Developing new multilayer polyelectrolyte charge mosaic membranes. **G. Vaseghi, G. Lipscomb***

14:00 – 1522. Removal of cyanide in solution using electrodeionization. **Y. Tian***, Y. Yang, X. Wu, Z. Fan, Z. Wu

14:20 – 1523. Recovery cyanide from cyanide-containing wastewater by selective-electroconcentration. **Y. Yang***, Y. Tian, Z. Fan, X. Wu, Z. Wu

14:40 – 1524. Charged membrane separations in hydraulic fracturing. **J.A. Hestekin**

15:00 – 1525. Preparation and characterization of methylmethoxysilane derived hydrophobic polymethylsilsesquioxane aerogel membranes for membrane distillation applications. **K. Tung***, C. Yang, C. Chuang, C. Ko, C. Chen, M. Huang, F. Hu

15:20 – 1526. Effect of membrane structure on membranes performance during membrane distillation. **R. Wickramasinghe, M. Malmali**

15:40 – 1527. Forward osmosis for water purification using impregnated membranes. **H. Lin***, S. Zhao, K. Huang, A. Balachandran

16:00 – 1528. Breakthrough water purification technologies based on nanofibrous membranes. **B.S. Hsiao***, B. Chu

16:20 – 1529. New approaches to membrane-based oil/water separations. **D. Jassby***, A. Dudchenko, X. Zhu, B. Chaudhary

Hawaii Convention Center
323A

Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294)

Organized by: T. Kato, M. Aizenberg, H. Kikuchi, S. Yu, H. Imai, C. Otsuki, C. Fraser, S. Kim

13:00 – 1530. Convergent evolution to engineering: Multifunctional biocomposite and biomimetic material. **D. Kisailus***

13:30 – 1531. Synthesis and characterisation of novel multidimensional fusion materials. **S. Valiyaveettil**

14:00 – 1532. Preparation of hollow capsules composed of *i*-PMMA/st-PMMA stereocomplex thin films by layer-by-layer assembly on macroporous silica gel. **H. Ajiro**, T. Ueyama, M. Akashi*

14:20 – 1533. Hierarchically structured assembly of inorganic nanosheets for tailored fusion materials. **M. Osada**, T. Sasaki

14:50 – 1534. Self-assembly of spherical and anisotropic polymer composite particles in biodevived cholesteric liquid crystal matrices. **C. Rosu***, J. Fu, E. Reichmanis, P.S. Russo

15:10 – 1535. Novel second order isotropic to nematic phase transition in hyper-swollen lyotropic liquid crystal driven by rod-sphere transition of micelles. **J. Yamamoto***, H. Jo, C. Ida, J. Lagerwall, G. Scallia

15:30 – 1536. Self-organizing organic-inorganic hybrid materials - from metal complexes to metal nanoparticles. **H. Eichhorn***, H. Taing, J. Yu, S. Salloum

16:00 – 1537. Biochemistry-enabled synthesis of functional nanomaterials. **E. Fong**

16:20 – 1538. Multicomponent tandem polymerizations of alkynes towards functional conjugated polymers. **R. Hu**, B. Tang

16:40 – 1539. Precise syntheses of ring-based vinyl polymers via ring-expansion living cationic polymerization. **M. Ouchi**

Hawaii Convention Center
326B

Aggregation Induced Emission: Materials and Applications (#444)

Organized by: M. Fujiki, B. Tang, B. Liu
Presiding: Q. Peng, B.Z. Tang, W. Tian

13:00 – 1540. Design, synthesis, and applications of aryl-substituted pyrroles with aggregation-induced emission characteristics. **Y. Dong***, X. Feng, J. Shi, B. Tong

13:30 – 1541. Aggregation-induced emission materials: The art of conjugation and rotation. **Z. Li**

14:00 – 1542. Preparation and biomedical applications of nanoprobe with aggregation-induced emission characteristics. **D. Ding***

14:20 break

14:20 – 1543. Design and syntheses of AIEgens with new structural motif. **R. Hu**, B. Tang

14:40 – 1544. Bright AIE nanoprobes with biocompatibility and photostability for functional bioimaging. **J. Qian***, Z. Zhu, A. Qin, B.Z. Tang

15:00 – 1545. Polysilane-triggered AIE-active explosive sensor based on FRET. **H. Sohn***

15:20 break

15:20 – 1546. Efficient nonfullerene organic solar cells based on new molecules with an AIE core. **H. Yan**

15:40 – 1547. New mechanistic insight into the aggregation-induced emission phenomenon. **B. Tang***

16:00 – 1548. Emission mechanisms and applications of phenylbenzoates based AIE compounds. **Y. Qian**, M. Cai, J. Li, W. Li, J. Ye, Z. Tu, L. XIE, G. Yang, W. Huang*

16:20 – 1549. Supramolecular engineering of metastable molecular aggregates for stimuli-responsive materials. **S. Yagai***

16:40 – 1550. AIE aggregate-amplified chemiluminescence resonance energy transfer. **C. Lyu**, L. Zhang, N. He, W. Guan

Saturday Evening

Hawaii Convention Center
Halls I, II, III

Dynamic, Reversible, and Self-healing Materials (#64)

Organized by: W. Skene, H. Otsuka, S. Rowan

Presiding: W. Skene

Poster Session

19:00 – 21:00

1551. Fixation and modification of dynamic covalent polymers: Insertion reactions of styrene derivatives into a disulfide-containing polyester. **Y. Nakai**, A. Takahashi, R. Goseki, H. Otsuka*

1552. Dynamic property of diselenide bond under visible light. **S. Ji**, W. Cao, Y. Yu, H. Xu*

1553. Structural reorganization of linear and cross-linked polymers using exchange reactions of diselenide bonds. **N. Suzuki***, T. Ohishi, R. Goseki, H. Otsuka

1554. Degradation of epoxy resins with disulfide bonds based on dynamic covalent chemistry. **A. Takahashi**, T. Ohishi, R. Goseki, H. Otsuka*

1555. Synthesis and mechanochromic property of crystalline polymers with diarylbenzofuranone. **S. Furukawa**, H. Oka, R. Goseki, H. Otsuka*

1556. Mechanochromic property of dynamic covalent polymers with diarylbenzofuranone functionality in the center of their structures. **H. Oka**, T. Sato, K. Imato, T. Ohishi, R. Goseki, H. Otsuka*

1557. Effect of self-healing performance based on paint system. **S. Park**

1558. Viscoelastic response of polyborosiloxanes gel triggered by reversible cross-linked networks. **M. Tang**, F. Jiang, Z. Wang*

1559. Synthesis and mechanochromic behavior of novel dynamic covalent polymers with multiarylate units. **T. Sumi**, R. Goseki, H. Otsuka*

1560. Rapid and reversible self-healing of bioactive double-wall carbon nanotube. **Y. Jung**

1561. Rapid synthesis of *m*-phenyleneimine macrocycle via melt-polymerization and thermoreversible conversion to linear oligomer based on DCC. **S. Kobayashi**, S. Hasegawa, H. Takei, Y. Nogawa, T. Matsumoto*

1562. Network reorganization of dynamic covalent polymer gels at ambient temperature. **K. Imato**, A. Takahashi*, H. Otsuka*

1563. Nanodoping of amino modified molecular sieves to enhance the dielectric performance of polymeric insulation by absorbing the degradation gases of electrical aging. **Y. Yang***, L. GAO, J. He

1564. Regulation of emulsion and vesicles by CO₂-switchable surfactants. **W. Qiao***

1565. Synthesis of new functionalized thermal-sensitive polymer. **F. Azemar**, D. Gomes Rodrigues, S. MONGE

1566. Synthesis and mechanoresponsivity of diarylbenzofuranone-containing cross-linked polymers prepared by sol-gel method. **T. Kosuge**, K. Imato, R. Goseki, H. Otsuka*

1567. Dynamic component exchange of conjugated materials. **M. Walesa-Chorab, W. Skene***

Hawaii Convention Center
Halls I, II, III

Current Polyurethane Science (#133)

Organized by: K. Kojo, S. Hsu, K. Wynne, Z. Ren, S. Yamasaki, G. Zhang

Poster Session

19:00 – 21:00

1568. Intramolecular hydroamination of polyallylurethanes with Pd-tethering macrocycle catalyst. **H. Iwasaki***, D. Aoki, H. Sugawa, T. Takata

1569. UV-curable waterborne polyurethane-acrylate containing sulfonic and carboxylic groups. **L. Wei**

1570. Comparative studies on anionic waterborne polyurethane dispersion based on salt group-containing diol as hydrophilic chain extender. **S. Fang***, L. Zhou, Z. Ren*, J. Zhang, X. Guo

1571. Novel polycaprolactone glycols bearing conjugated triene for biodegradable polyurethane: Structure and crystallization behavior. **G. Zhang**, X. Guo, H. Wang, Z. Ren

Hawaii Convention Center
323B

Advanced Membrane Separations (#262)

Organized by: R. Wickramasinghe, K. Tung, H. Chen, S. Husson
Presiding: H. Chen, S.M. Husson

19:00 – 1572. Multimodal membranes for protein purifications at high ionic strength. **J. Wang**, S.M. Husson

19:20 – 1573. Understanding the effect of salt ions on protein adsorption in novel responsive hydrophobic interaction membrane chromatography. **X. Qian***, Z. Liu, R. Wickramasinghe

19:40 – 1574. TiO₂ based enzymatic membranes and membrane reactors. **J. Hou**, Y. Wang, N.A. Lee, V. Chen*

20:00 – 1575. Lactic acid production in a membrane bioreactor system with thermophilic *Bacillus coagulans*: Fouling analysis and process control with an innovative optical sensor. **R. Fan**, M. Ebrahimi, H. Quitmann, P. Czermak

20:20 – 1576. Selective enantiomer separation by pertraction and pervaporation with chiral polymeric membranes. **P. Izak***, J. Zitka, L. Brozova, P. Sysel, H. Vychodilova, L. Stastna-Cervenka, S. Horvorka

20:40 – 1577. Fractionating complex protein lignin process streams by tubular ceramic membranes. **N. Busse**, M. Kraume, P. Czermak

Hawaii Convention Center
323A

Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294)

Organized by: T. Kato, M. Aizenberg, H. Kikuchi, S. Yu, H. Imai, C. Otsuki, C. Fraser, S. Kim

19:00 – 1578. Fusion between microfabrication and biomaterials: Application for artificial cell membranes and biomimetic microfluidics. **R. Kawano***

19:15 – 1579. Producing coloured materials with amorphous arrays of black and white colloidal particles. **Y. Takeoka***

* Principle Author

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- 19:30 – 1580.** Dye-sensitized solar cells based on self-assembled liquid-crystalline electrolytes. **D. Höglberg**, B. Soberats, S. Uchida, M. Yoshio, L. Kloo, H. Segawa, T. Kato*
- 19:45 – 1581.** Design of bicontinuous cubic liquid-crystalline assemblies using ionic liquids as building block. **T. Ichikawa**, T. Matsumoto, A. Okafuji, K. Fujimura, M. Yoshio, T. Kato, H. Ohno*
- 20:00 – 1582.** Supramolecular nanoparticle carrier self-assembled from cyclodextrin and adamantane-functionalized polyacrylates for tumor-targeted drug delivery in both in-vitro and in-vivo model. **C. Ang**, S. Tan, X. Wang, Q. Zhang, S. Subramanian Tamil, N. Tan, Y. Zhao*
- 20:15 – 1583.** Nanofusion materials for photodynamic therapy by near infrared irradiation. **K. Katagiri***, I. Shimizu, M. Narahara, K. Tomita, A. Ikeda, K. Inumaru
- 20:30 – 1584.** Linearly polarized emission of lanthanide complexes with layer arrangement in the Langmuir-Blodgett film. **A. Ishii***, N. Goto, M. Hasegawa
- 20:45 – 1585.** Silica nanoarchitectures synthesized via a block copolymer-mediated approach. **A. Sugawara-Narukati***, S. Zhou, S. Tsuboi, T. Okubo, Y. Oda, K. Landenberger, A. Shimojima, S. Aoshima

Sunday Morning

Hawaii Convention Center
324

Dynamic, Reversible, and Self-healing Materials (#64)

Organized by: W. Skene, H. Otsuka, S. Rowan
Presiding: H. Otsuka, W. Skene

8:00 – 1586. Injectable magnetic hydrogels containing embedded thermoresponsive microgels facilitating “on-demand” drug release. S. Campbell, D. Maitland, T. Hoare*

8:15 – 1587. Mussel-inspired, self-healing poly(dopamine methacrylate)/polyurethane blends and nanocomposites. S. Song, Y. Tang, X. Qu, Z. Yang, J. Huang*

8:30 – 1588. Artificial spores: Cytoprotective and degradable nanocoating of mammalian cells. **J. Lee***, S. Yang, I. Choi

8:45 – 1589. Malleable and self-healing polymer networks based on dynamic imine bond exchange. **A. Chao**, D. Zhang*

9:00 – 1590. UV light triggered self-healing composites based on ZnO-graphene quantum dots. **S. Ahn***, K. Park, B. Moon

9:15 – 1591. Structurally dynamic assemblies of stimuli-responsive polymers. C. Deng, J. Cash, W. Brooks, T. Kubo, B.S. Sumerlin*

9:45 coffee

10:00 – 1592. Glucose-Induced self-healable polyurethanes. **M.W. Urban**

10:30 – 1593. Thermoresponsive and self-healing polymers based on guest–host interactions. Y. Jia, J.X. Zhu*

10:45 – 1594. Study on electrochemical redox responsive supramolecular self-healing hydrogels. L. Peng, H. Zhang, J. Yuan*

11:00 – 1595. Mechanically interlocked polymer networks viaradical-radical interactions. **Z.S. Kean**, J.F. Stoddart*

11:15 – 1596. Thermostimulated reversible interconversion between a macrocycle and the linear oligomers. **T. Matsumoto***, S. Kobayashi, S. Hasegawa

11:30 – 1597. Thermotropic transformation of polyacetylene’s main-chain conformation having tunable critical one-handed spiraling temperature. **I. Liu**, W. Wang, Y. Wang, C. Zhang, T. Aoki, Y. Okamoto

11:45 – 1598. Hypervalent iodine(III) compounds in the synthesis of dynamic polymers with controlled macromolecular architectures. **N.V. Tsarevsky***, H. Han

Hawaii Convention Center
326A

Radical Polymerization Kinetics and Process Modeling (#92)

Organized by: R. Hutchinson, G. Russell, P. Zetterlund, E. Saldívar-Guerra

8:00 Introductory remarks

8:05 – 1599. About the relevance of detailed elementary kinetics in modern LDPE product development. **M. Busch**

8:35 – 1600. Exploring the evolution of molecular architecture in free radical copolymerizations with divinyl monomers using Monte Carlo kinetic simulations with restricted chain diffusion. **D.C. Sundberg***, A. Tripathi, J. Tsavalas

9:05 – 1601. Crosslinking polymerization in resin applied in laser stereolithography. **A.N. Nikitin***

9:25 – 1602. Controlled radical polymerization of dimethacrylate networks. **E.M. Redline***, G. O’Bryan, D.S. Bolintineanu, J. Lane

9:45 Break

10:00 – 1603. Kinetics and modeling of the radical polymerization of ionized monomers in aqueous solution. **P. Drawe***, M. Buback, I. Lacik

10:20 – 1604. Acrylamide copolymerization with cationic monomers in aqueous solution: Experimental and modeling study. **D. Cuccato***, G. Storti, M. Moribelli

10:40 – 1605. Mathematical modeling of nitroxide mediated emulsion polymerization via a robust semibatch process. **E. Saldívar-Guerra***, A. Cano-Valdez, R. González-Blanco, M. Cunningham

11:00 – 1606. Fast completion of radical polymerization by heating to ultrahigh temperature under pressure. **K. Kinoshita**, S. Deguchi

Hawaii Convention Center
323C

New Frontiers in Polymer Crystallization (#96)

Organized by: W. Hu, A. Toda, C. Li
Presiding: B.S. Hsiao, T. Kanaya

8:00 Green Polymers

8:00 – 1607. Crystallization processes of poly(L-lactic acid). **B. Lotz***

8:20 – 1608. Structure characterization of cellulose nanofibers and microfibrils. **B.S. Hsiao***, B. Chu, Y. Su

8:40 – 1609. Spherulite crystallization of cellulose from its concentrated solutions in ionic liquids. **J. Zhang**

9:00 – 1610. Crystallization process of eco-friendly polyurea. **G. Matsuba**, Y. Chonan, K. Nishida, T. Kanaya, T. Itoh, T. Akizuki

9:20 – 1611. Kinetics of strain-induced crystallization in cross-linked natural rubber. **M. Tosaka***

9:40 – 1612. Flow-induced crystallization of a long chain aliphatic polyamide in multiple flow fields: A novel anisotropic structure and formation mechanism. **X. Dong***, Y. Gao*, D. Wang

9:55 Break

10:05 Stretch- or Flow-induced

10:05 – 1613. Nano-oriented crystals (NOCs) of PET in elongational crystallization. **M. Hikosaka***, K. Okada, Y. Tanaka, H. Masunaga

10:25 – 1614. Effect of solvent size on aggregation and crystallization of polymers. **Q. Xue**

10:45 – 1615. Effects of molecular weight in flow- and deformation-induced polymer crystallization. **T. Kanaya***

11:05 – 1616. Molecular simulations of di-block copolymers performing fibril crystal growth in solutions. **W. Hu***, R. Shu, A. Eman, L. Zha

11:25 – 1617. Role of entanglement species in the formation of shish-kebab – effect of blend ratio and molecular weight in cyclic and linear polyethylene blend. **S. Yamazaki***

11:45 – 1618. Molecular simulations of shish-crystal formation in polymer shear flow. **Y. Nie**, W. Hu*

Hawaii Convention Center
325B

Current Polyurethane Science (#133)

Organized by: K. Kojo, S. Hsu, K. Wynne, Z. Ren, S. Yamasaki, G. Zhang

Presiding: Y. Higaki

8:00 – 1619. Effects of chemical structure of diisocyanate on a microdomain structure and physical property of polyurethane elastomers. **K. Kojo**, S. Nozaki, A. Takahara

8:30 – 1620. Healing behavior of a microphase-separated structure of segmented polyurethane after mechanical deformation. **S. Nozaki**, K. Kojo*, A. Takahara*

8:55 – 1621. Relationship of branched structure and conductive property of carbonate oligomer-based electrolytes. **K. Kaetsu**, T. Ohishi, T. Hirai, Y. Higaki, K. Kojo*, A. Takahara*

9:20 Break

9:35 – 1622. Cross-linkable ionic and non-ionic polyurethanes from renewable tung oil. **Z. Ren***

9:35 – 1623. Synthesis and properties of hydroxylated tung oil based waterborne anionic polyurethanes dispersion. **L. Jiang**, Z. Ren, Y. Fu, B. Ren, C. Zhu

11:05 – 1624. Crosslinkable waterborne polyurethane protective coatings. **M. Rahman***

11:30 – 1625. Force sensitive waterborne polyurethane with shape memory properties. **Q. Zhang***

11:55 Closing Remarks

Hawaii Convention Center
325A

Macromolecular Self-Assembly for Smart Biomaterials (#196)

Organized by: S. Thayumanavan, L. Dai, J. Ryu
Presiding: J. Ryu

8:00 – 1626. Supramolecular coordination assisted crosslinking of polymer networks into anisotropic assemblies. **L. Dai**, C. Yuan

8:25 – 1627. Nanoparticle-stabilized capsules as therapeutic delivery agents for treatment of breast cancer. J. Hardie, M.A. Mingroni, E. Tetraulx, P. Ghazi, V.M. Rotello, M.E. Farkas*

8:50 – 1628. ROS responsive Se/Te-containing polymers. **H. Xu**

9:15 – 1629. Self-assembly as a design principle in the development of binary anti-thrombotic and antimicrobial coating with exceptional properties. **J. Kizhakkedathu***, Y. Mei, K. Yu

9:40 – 1630. Direct correlation of molecular structure with self-assembled nanostructures and biological functions for a new family of dendrized peptide amphiphiles designed for safe and effective siRNA delivery. **Z.M. Guan***

10:05 Break

10:15 – 1631. Functional nanomaterials through self-assembly of reactive polymers. **A. Sanaya***

10:40 – 1632. Drug-initiated method: a convenient approach for the synthesis of efficient polymer prodrug nanoparticles. **S. Harrisson**, D. Bui, A. Maksimenko, P. Couver, J. NICOLAS*

11:00 – 1633. Amphiphilic star block copolymer-based multifunctional micelles for synergistic photoactuated drug delivery and MR imaging. **G. Zhang**, N. Chen

11:20 – 1634. PAMAM dendron-lipid assemblies as stimuli-responsive drug delivery systems. **K. Kono***, Y. Hirai, Y. Yamamoto, E. Yuba, A. Harada

Hawaii Convention Center
327

Cyclic and Topological Polymers (#248)

Organized by: Y. Tezuka, S. Grayson, M. Monteiro
Presiding: S. Grayson

8:00 – 1635. Topology-directed diffusion and relaxation of polymers revealed by single-molecule imaging. **S. Habuchi***

8:30 – 1636. Anomalous self-diffusion in asymmetric ring-linear blends. **S. Shanbhag***

8:50 – 1637. Understanding and characterizing the effect of nanoscale confinement on glass transition temperature and film dewetting of macrocyclic polystyrene. **L. Zhang**, R. Elupula, S. Grayson*, J. Torkelson*

9:10 – 1638. Diffusion coefficient and the mean-square radius of gyration for various topological polymers through the quaternion algorithm. **T. Deguchi***, E. Uehara

9:40 – 1639. Scattering function of wormlike rings. **D. Ida***, R. Tsubouchi, T. Yoshizaki

10:00 Break

10:10 – 1640. Controlled self-assembly behaviors of asymmetric ring and star polymers in bulk and solution states. **M. Ree***, Y. Kim, K. Heo, B. Ree, Y. Kitazawa, D. Kawato, Y. Satoh, T. Isono, T. Yamamoto, T. Satoh, T. Kakuchi

10:40 – 1641. Linear-cyclic topological transformation for switching the properties of polymeric materials. **T. Yamamoto***, Y. Sugai, S. Asai, Y. Tezuka

11:00 – 1642. Synthesis of carbon-dioxide-derived cyclic poly(propylene carbonate)s. **S. Honda**, H. Sugimoto

11:20 Closing Remark

Hawaii Convention Center
323B

Advanced Membrane Separations (#262)

Organized by: R. Wickramasinghe, K. Tung, H. Chen, S. Husson
Presiding: K. Tung, R. Wickramasinghe

8:00 – 1643. Water vapor and CO₂ permeation through amine-containing facilitated transport membranes for H₂ purification and CO₂ capture. **W. Ho**

8:20 – 1644. Amino acid ionic liquid-based tough gel membrane for CO₂ capture. **H. Matsuyama***, E. Kamio, F. Moghadam

8:40 – 1645. Polymers of intrinsic microporosity for use as molecular sieve membranes. **N. McKeown***, M. Carta, I. Rose, C.G. Bezu, R. Malpass-Evans, P. Paola Bernardo, J. Jansen, G. Clarizia

9:00 – 1646. Ultrapermeable polymers of intrinsic microporosity (PIMs) based on benzotriptycene. **I. Rose**, M. Carta, C.G. Bezu, P. Paola Bernardo, J. Jansen, G. Clarizia, N. McKeown

9:20 – 1647. Ultrapermeable polymers of intrinsic microporosity based on spirobifluorenes. **C.G. Bezu**, M. Carta, J. Jansen, P. Paola Bernardo, G. Clarizia, N. McKeown

* Principle Author

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9:40 – 1648. Permeation of oil-in-water emulsions through membrane: Numerical simulation using phase-field model.

Y. Mino, Y. Kagawa, T. Ishigami, H. Matsuyama*

10:00 – 1649. Improving selectivity of polyamide composite membranes: principles and implementation. **V. Freger***

10:20 – 1650. Demonstration project of Integrated membranes process to remove organic pollutants for municipal drinking water. **H. Chen***, C. Zhang, S. Chen, X. Chen, L. Zhang

10:40 – 1651. Addressing separation challenges through industry-university collaborative research centers. **A. Greenberg***, R. Noble, K. Sirkar

11:00 – 1652. Some lateral thinking in membrane chromatograph. **R. Ghosh***, P. Madadkar, R. Sadavarte

Hawaii Convention Center
323A

Fusion Materials: Functional Self-Organized Materials Consisting of Fused Organic and Inorganic Components (#294)

Organized by: T. Kato, M. Aizenberg, H. Kikuchi, S. Yu, H. Imai, C. Otsuki, C. Fraser, S. Kim

8:00 – 1653. Luminescent fusion materials for optoelectronics devices. **T. Yasuda***

8:20 – 1654. High performance selenium-bridged V-shaped organic semiconductors exhibiting unique structural transition and high solution-processability.

T. Okamoto*, C. Mitsui, M. Yamagishi, M. Mitani, T. Kato, H. SATO, A. Yamano, J. Takeya

8:40 – 1655. Engineering nanoelectronic devices with the aid of molecular chemistry. **D. Kiriyama**, A. Javey

9:05 – 1656. Photoinduced macroscopic morphological transformation of an amphiphilic diarylethene assembly: Reversible dynamic motion. **K. Higashiguchi***, G. Taira, J. Kitai, T. Hirose, K. Matsuda

9:25 – 1657. (Photo)electrochemistry as a powerful tool in the rational design of hybrid organic/inorganic semiconductor assemblies. **C. Janaky***, G. Samu, K. Rajeshwar

9:45 – 1658. Photocontrol of molecular alignment in liquid crystal systems.

A. Shishido*, J. Wang, Y. Aihara, M. Kinoshita

10:05 – 1659. Surface functionalization of polystyrene cell culture plate with biomimetic apatite for preparation of artificial bone marrow niches. **K. Iijima**, R. Suzuki, N. Kiyoaka, M. Hashizume*

10:25 – 1660. Genetic control of magnetite crystal shapes in magnetotactic bacteria. **A. Arakaki**, A. Yamagishi, M. Tanaka, T. Matsunaga

10:40 – 1661. Development of pyrazine-2-carboxylate titanium complexes using a water-soluble titanium complex.

M. Kobayashi*, T. Okuhara, H. Kato, S. Sato, M. Kakihana

10:55 – 1662. Crystallization of calcium carbonate in lyotropic hexagonal liquid crystal phases. **H. Higuchi**, K. Nagaoka, M. Shimoda, Y. Okumura, T. Nishimura, T. Kato, H. Kikuchi*

11:10 – 1663. Glassin, a silica polycondensation directing protein from the siliceous skeleton of the hexactinellid sponge *Euplectella*. **K. Shimizu***, T. Amano, J. Arima

11:25 – 1664. Development of organic/inorganic fusion materials using oriented chitin matrices as templates. **T. Nishimura***, T. Kato*

11:40 – 1665. Hydroxyapatite formation from calcium phenyl phosphate in a solution mimicking human blood plasma: Effects of alkaline phosphatase addition.

C. Ohtsuki*, A. Mio, T. Ujiyama, A. Sugawara-Narutaki, T. Yokoi

11:55 Closing Remarks

Hawaii Convention Center
326B

Aggregation Induced Emission: Materials and Applications (#444)

Presiding: C. Lyu, K. Tanaka, M. Zhu

8:00 – 1666. General synthetic approach toward geminal-substituted tetraarylethene chromophores with aggregation induced emission. **M. Zhu**

8:30 – 1667. Diketopyrrolopyrrole (DPP) dye with aggregation-induced red/NIR emission for in vivo two-photon fluorescence imaging. **Y. Gao**, **J. Hu**, H. TIAN

9:00 – 1668. Regulation of aggregation-induced emission properties of group 13 elements-containing compounds and their applications as optically-functional materials. **K. Tanaka***, Y. Chujo

9:30 break

9:30 – 1669. Origin of aggregation induced emission in BF_3 -hydrazones (BODIHYs) - a novel class of fluorescent molecular rotors. **I. Aprahamian***, H. Qian, M. Lipack

9:50 – 1670. Development of photofunctional liquid crystals controlled by assembled structures by external stimuli.

T. Kato*

10:10 – 1671. Mechanofluorochromism and aggregation induced emission observed for 4-(diarylamino)benzaldehyde analogs. **K. Mizuguchi**, K. Okoshi, S. Manabe, M. Kurita, M. Momma, H. Nakano*

10:40 break

10:40 – 1672. Mass-less spinning photon swaps hand of luminous helical polymer aggregates. **M. Fujiki***

11:00 – 1673. Theoretical insights into the mechanism of aggregation-induced emission. **Q. Peng**

11:20 – 1674. Highly photoluminescence electrospun nanofiber mats embedded with AIE-active diaryl benzene derivatives. **F. Anariba***, M. Sobhan

11:40 – 1675. Insight into the exploration of energy modulations of TPE and RhB in bichromophoric systems. **R. Singh**, A.K. Dwivedi, H. Lin*

ORGN

Area 4 – Organic

Tuesday Morning

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

Prospects for Flow Chemistry (#29)

Organized by: J. Yoshida, T. Jamison, D. Kim, M. Organ

Presiding: C. Kappe, J. Yoshida

8:00 – 1. Use of continuous flow technology to harness hazardous chemistries and process conditions. **C. Kappe***

8:25 – 2. Flowing safely: Synthesis with hazardous chemicals. **T. Wirth**

8:50 – 3. On-demand diazo reagents: In-flow generation and purification.

E. Levesque*, S.T. Laporte, S. Vanier, A.B. Charette

9:05 – 4. Generation of anhydrous diazo-methane using a Teflon AF-2400 membrane. **B. Gutmann**, C. Kappe

9:20 – 5. Monophasic generation and reaction of diazomethane in in-flow cyclopropanation. **A. Evans***, C. Ayoub

9:35 – 6. Flash chemistry enables chemoselective reactions of difunctional electrophiles with functionalized allylithiums.

A. Nagaki, S. Ishiiuchi, K. Imai, J. Yoshida*

9:50 – 7. Liquid-liquid microflow for the Beckmann rearrangement of cyclohexanone oxime. J. Zhang, K. Wang, Y. Lu, **G. Luo***

10:15 – 8. Nucleophilic addition to nitrones using flow microreactors. **Y. Arakawa**, S. Ueta, K. Minagawa, Y. Imada*

10:30 – 9. Integrated reactions based on the sequential additions to conjugated imines. **M. Shimizu***, I. Mizota

10:45 – 10. Flow synthesis of (E)-(S)-3-hydroxy-7-tritylthio-4-heptanoic acid, a key component of the natural product cyclodepsipeptide HDAC inhibitors.

M. Yoshida, H. Otaka, K. Umeda, T. Doi*

11:00 – 11. [2+2+1] Cocyclization using alkenes, diketones, and bis(iodozincio-)methane. **R. Haraguchi**, S. Matsubara*

11:15 – 12. Study of scaled continuous flow production of metal-organic frameworks.

M. Rubio Martinez*, T. Hadley, K. Constanti, M. Batten, A. Polyzos, K. Lim, M.R. Hill

11:30 – 13. Synthetic study of glycans using integrated reaction systems. **F. Koichi***, Y. Manabe

11:45 – 14. Controlling differentiation of mesenchymal stem cells with microfluidic flows. **H. Shum***, W. Lai

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

Molecular and Supramolecular Photochemistry (#71)

Organized by: J. Sivaguru, W. Chung, C. Bohne, c. Tung, M. Sakamoto, V. Ramamurthy

Presiding: V. Ramamurthy

8:00 Turo Symposium / Opening remarks

8:05 – 15. Photoinduced charge separation in DNA. **F.D. Lewis***

8:35 – 16. Photoresponsive artificial muscle model unit in microenvironment with supramolecular interaction and cooperation. **H. Inoue***

9:05 – 17. Catalysis by niobium-oxide nanostructured materials. **J. Scaino**, G.L. Hallett-Tapley, S. Impellizzeri, C. Fasciani, S. Simoncelli, J. Netto Ferreira, M. Marin

9:35 Break

9:50 – 18. Cross-coupling hydrogen evolution reactions initiated by photoinduced electron transfer. **C. Tung***, Q. Meng, X. Li, Y. Zheng, P. Ye, K. Feng, B. Chen, L. Wu

10:20 – 19. Supramolecular organization of photoactive metal complexes in 1- and 3D. **A.A. Marti***, A. Saha, K. Huang, C. Jiang, D.M. Guld, K. Dirian, D. Jain, Z. Panos, T. Hanna, M. Hernandez-Rivera

10:50 Break

11:05 – 20. Novel strategy of supramolecular asymmetric photocirogenesis with tailor-made biopolymers as chiral reaction media. **T. Wada***, M. OKUJI, H. SASAKI, Y. Ikeda, S. SAKAMOTO, Y. Araki*, M. NISHIJIMA, K. TSUMOTO, Y. NAGASAKI, Y. Inoue

11:35 – 21. Light harvesting vesicular scalfold reduces the rate of charge recombination in the presence of an electron donor. **M. Hariharan***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74)

Organized by: R. Danheiser, T. Fukuyama, M. Lautens

Presiding: R. Danheiser

8:00 Introductory Remarks

8:05 – 22. Exploiting the versatile N-O bond: Rapid synthesis of NH-aziridines and carbazoles. **L. Kurti***

8:25 – 23. Synthetic studies on lycopanthine. **A. T. Fukuyama***, Y. Ochi, S. Yokoshima

9:05 – 24. Total synthesis of polycyclic alkaloids, lundurines, and grandilodine.

A. Nishida*, M. Nakajima, S. Arai

9:45 – 25. Utility of bimolecular free-radical reactions in fragment coupling.

L. Overman*

10:25 – 26. Chemical synthesis of secondary metabolites. **R.A. Shenvi**

11:05 – 27. Enabling reactivity of neutral aminyl radicals for the synthesis of complex alkaloids. **J.L. Stockill**

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Homogeneous Gold Catalysis: Methods, Theories and Applications (#192)

Organized by: L. Zhang, H. Ohno, R. Liu
Presiding: H. Ohno

8:00 opening remarks-highly efficient gold catalysis

8:10 – 28. Difunctional ligands open up gold reactivity: Toward new avenues in catalysis? **G. Bouhadir, A. Amgoune, D. Bourissou***

8:30 – 29. Structure and reactivities of gold complexes synthesized from alkylene-functionalized ligands. **N. NISHINA**, H. TAKEMOTO, E. Hasegawa, F. KIMURA

8:50 – 30. Hydrogen bonding basicity and gold catalysis: A synergistic combination. **G.B. Hammond***, B. Xu

9:10 – 31. Homogeneous catalysis involving dinuclear gold species. **S. Hashmi**

9:45 break

10:00 – 32. Mechanistic study of gold mediated intramolecular alkene addition reactions. **A.C. Jones***, Y. Zhu

10:20 – 33. Development of novel gold-catalyzed migratory transformations.

V. Gevorgyan*

10:50 – 34. Accessing nitrenoid-based dipole reactivity using gold catalysis.

P. Davies*

11:10 – 35. Intermediate-based approach to new reaction discovery in gold catalysis.

S. Shin

11:40 – 36. Gold-catalyzed ring expansion of 2-propargyl-beta-tetrahydrocarbolines.

S. Wang*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Molecular Function of Natural Products: Advances towards Chemical Biology (#237)

Organized by: M. Ueda, B. Miller, K. Irie, B. Miller, B. Miller, C. Lin, T. Oishi, C. Forsyth, H. Lee

Presiding: M. Ueda

8:00 – 37. Total synthesis, stereochemical revision, and biological evaluation of lycyluloside B, a marine macrolide glycoside. **H. Fuwa***, Y. Okuaki, N. Yamagata, M. Sasaki

8:15 – 38. Third generation photo-cross-linked small-molecule affinity matrix enabling quantitative analysis of the photo-cross-linked small molecules and their target purification. **N. Kanoh***, T. Suzuki, T. Okamura, Y. Iwabuchi

8:30 – 39. Target-selective photodegradation of proteins in chemical biology.

K. Toshima*

8:45 – 40. Synthesis of fluorescent ligand for visualization of native ionotropic glutamate receptors. **T. Shinada***, Y. Ohnue

9:00 – 41. Extraction of antiproliferative activity from pleiotropic debrisoquine-alkaloid, a potent tumor promoter and a highly inflammatory principle isolated from sea hare. **K. Irie**, M. Kikumori, R.C. Yanagita, H. Tokuda

9:20 – 42. Turn-on fluorescent affinity labeling using a small bifunctional O-nitrobenzodiazepine unit. **M. Sodeoka***

* Principle Author

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9:40 – 43. Identification and mechanistic analysis of novel antibiotic "Lysocin E".
K. Sekimizu, H. Hamamoto

10:00 – 44. Discovery and target identification of pyrrolactone, a fungal metabolite. H. OSADA, Y. Futamura, T. Nogawa

10:30 – 45. Chemical biology fantasia.
D. Uemura*

11:15 – 46. Function through synthesis-informed design: New therapeutic leads for Alzheimer's disease, cancer, and HIV/AIDS eradication. P.A. Wender*

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Frontiers of Chirality in Organic Chemistry (#286)

Organized by: J. Canary, N. Berova, E. Yashima, M. Hyun, T. Shibata, T. Asahi, C. Welch, S. You
Presiding: J. Canary, E. Yashima

8:00 Introduction

8:05 – 47. Reconfigurable chiral copper complexes: Ambidextrous catalysis.
J. Canary*

8:35 – 48. Double-stranded helical foldamers as unique chiral materials. E. Yashima

9:05 – 49. Chirality of nanoscale gold particles and clusters. T. Bürgi*

9:35 – 50. Squeezable tubes with tunable chirality from self-assembly of macrocycle amphiphiles. M. Lee*

10:05 Break

10:15 – 51. Chiral inorganic mesostructured films with multi-optical activity. S. Che

10:45 – 52. Control of the chirality and helicity of artificial duplex by sequence design. H. Asanuma*, K. Murayama, H. Kashida

11:00 – 53. Redox-triggered chiroptical molecular switches based on the helicates of oligopyrrole- α,ω -dimers. J. Setsune*

D. Saito, K. Imamura

11:15 – 54. Helical (supra)molecular chirality in tetraphthalvalenanes and derived materials. N. Avarvari*

11:30 – 55. Elastic switching of chiral foldamers in response to acid/base and redox stimuli. H. Miyake*

11:45 – 56. Construction and evaluation of planar chiral π -conjugated system based on a tetrasubstituted [2,2]paracyclophane framework. M. Gon*, Y. Morisaki, Y. Chujo

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Supramolecular Chemistry at the Interface of Materials, Biology, and Medicine (#300)

Organized by: S. Zimmerman, Z. Li, K. Kim
Presiding: K. Kim

8:00 – 57. Molecular recognition of repeating RNA and DNA sequences by small molecules. S. Zimmerman*, L. Nguyen, L. Luu, J. Serrano, J. Lee, C. Wong

8:30 – 58. Sequence-targeted invasion of DNA and RNA G quadruplexes by peptide nucleic acid. B. Armitage*

9:00 – 59. Stimuli-responsive synthetic ion channels. T. Muraoka*, K. Kinbara*

9:20 – 60. Ligand binding to hex 69 of 23S rRNA. C.S. Chow*

9:50 – 61. New isomeric fluorescent nucleosides for studying RNA-based processes. Y. Tor

10:20 – 62. Smart materials from cyclodextrin polyrotaxanes. G. Wenz

10:40 – 63. Recent progress on fluorescent imaging probes for reactive oxygen species and GSH. J. Yoon*

11:10 – 64. Macromolecular recognition: Interaction of cyclodextrins with polymer side chains. A. Hashidzume, A. Harada*

11:30 – 65. Achieving isothermal DNA self-replication by dialing in destabilization. J. Gibbs-Davis, B. Alladin-Mustan, A. Kausar, C.J. Mitrani

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Nanomaterials as Catalysts for Green Chemistry (#313)

Organized by: A. Moores, Y. Uozumi, C. Li, R. Varma

8:00 Break

8:20 – 66. Hydrogen production by methanol steam reforming on ZnO nanowire supported Pd single atoms and nanoparticles. J. Liu*, J. Xu, D. Yuchi

8:40 – 67. Controlling catalytic selectivity via design of the near-surface environment. J. Medlin*

9:00 – 68. Methyltrioxorhenium supported on mesoporous Al₂O₃ promoted with ZnCl₂ as a green heterogeneous catalyst for methyloleate self-metathesis: Reaction kinetics. K. Belkacemi*, S. Pillai, S. Hamoudi

9:20 – 69. Effective transformation of biomass into value-added chemicals over well-defined metal catalysts at nano and sub-nano dimensions. N. Yan*

9:40 – 70. Hydrogen bond promoted reactions for green process innovation. Z. Suojiang*

10:00 Break

10:20 – 71. Palladium meets gold: Peculiar activity of bimetallic gold/palladium alloy nanoclusters. H. Sakurai

10:40 – 72. Magnetic nanocatalysts in sustainable organic syntheses and transformations. R.S. Varma

11:00 – 73. "Coordinating" nanoparticle catalyst: Synthesis and application. Z. Li, P. Sun, C. Xia, F. Li

11:20 – 74. Nanoconfined metal complex catalysts and their application in activation of alkanes to alcohols. A. Karkamkar*

11:40 – 75. Co-N-C: Efficient and durable noble metal-like catalysts for selective oxidative and hydrogenative transformations. L. ZHANG, W. LIU, A. Wang*, T. Zhang*

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

Mechanochemistry and Solvent-free Synthesis (#322)

Organized by: T. Friscic, E. Juaristi, C. Raston

8:00 – 76. Use of D-mandelic acid as chiral additive in the Michael addition reaction organocatalyzed by (1S,4S)-2-tosyl-2,5-diazabicyclo[2.2.1]heptane under solvent-free conditions. E. Juaristi*, C. Avila-Ortiz

8:20 – 77. Mechanochemical steps to solvent-free porphyrin synthesis. T. Hamilton*

8:40 – 78. Mechanochemical solvent-free reaction for the synthesis of unique derivatives of fullerenes. K. Komatsu*

9:05 – 79. High pressure accelerated/Induced organic reaction in crystalline state. Y. Ma, X. Meng

9:25 – 80. Mechanochemistry as a route to novel forms of multicomponent crystals. L. Loots, J.P. O'Connor, T. le Roex, D.A. Haynes*

9:45 Coffe Break

9:50 – 81. Continuous flow vortex fluidics: High shear control of chemical reactivity and selectivity. C. Raston*

10:10 – 82. Mechanochemical insight into organometallic synthesis: What role does the solvent play?. N. Rightmire, D.L. Bruns, T.P. Hanusa*

10:30 – 83. How can we optimize the mechanochemical processes at the surface of organic solids for affordable materials fabrication?. M. Senna

10:55 – 84. Mechanochemical reactions of phosphazanes. f. garcia, X. Shi

11:15 – 85. Mechanochemistry and its applications: From organic synthesis of active pharmaceutical ingredients to catalysis. E. Colacicno*

11:40 – 86. Redox-promoted self-assembly of metal-organic materials in the solid state: Applications in materials synthesis and bulk-metal oxidation. M. Glavinovic, F. Qi, A. Katsenis, T. Friscic, J. Lumb

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Carbenes and Carbenoids in Organic Synthesis (#362)

Organized by: K. Scheidt, M. Murakami, R. Chi

Presiding: Y. Chi, M. Murakami, K. Scheidt

8:00 – 87. Development of chemo- and stereoselective carbene-catalyzed reactions. M. Gravel

8:25 – 88. NHC-catalyzed resolution and de-symmetrization of alcohols and beyond. Y. Zhao*, S. Lu, S. Poh

8:50 – 89. Highly stereoselective radical cyclopropanation of alkenes with diazoniums via cobalt(II)-based metalloradical catalysis. J. Wang*, X. Xu, S. Zhu, X. Cui, L. Wojtas, P. Zhang*

9:15 – 90. Asymmetric synthesis using ylides generated from Rhodium carbenoids in combination with chiral Ni(II), Zn(II), and Cu(II) catalysts. H. Sugai*, T. Bandou, T. Yoshida

9:40 Break

10:00 – 91. New reactions of "Donor/Donor" carbenoids. K.N. Lamb, R.A. Squitieri, N.P. Burlow, G.P. Shearn-Nance, J.T. Shaw*

10:25 – 92. N-sulfonyltriazoles as useful precursors to donor/acceptor carbenes. H.M. Davies*

10:50 – 93. Gold-catalyzed oxidative cyclizations, cycloaddition, and 1,2-difunctionalizations of alkynes via gold carbene intermediates. R. Liu

11:15 – 94. Acyl anion equivalent free enantioselective catalysis with N-heterocyclic carbenes. D.W. Lupton

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Cognizance of Endangered Elements for Organic Synthesis (#415)

Organized by: H. Tsuji, S. Zhu, G. Konishi, C. Luscombe, L. Campeau
Presiding: L. Campeau, S. Zhu

8:00 Introductory Remarks

8:10 – 95. Cu-, or Fe-catalyzed C-H/C-C bond oxygenation and nitration reactions. N. Jiao

8:40 – 96. Homogeneous nickel-catalyzed asymmetric hydrogenation of olefins. M. Shevlin

9:00 – 97. Cobalt catalysis for C-H functionalization. N. Yoshikai

9:30 Break

9:45 – 98. Alternatives to rare late transition elements in C-H and C=C activation reactions. F. Michael*

10:15 – 99. Vinylic and allylic C-F bond activation via nickel-catalyzed fluorine elimination. T. Fujita, T. Ichitsuka, Y. Watabe, T. Arita, J. Ichikawa*

10:35 – 100. Regioselective trifluoromethylation of 6-membered heteroaromatic compounds. Y. Kuninobu*, T. Nishida, M. Nagase, H. Ida, M. Kanai*

10:55 – 101. Carboperoxidation of alkenes and synthetic applications. Z. Li

Tuesday Afternoon

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

Prospects for Flow Chemistry (#29)

Organized by: J. Yoshida, T. Jamison, D. Kim, M. Organ
Presiding: T.F. Jamison, I. Ryu

13:00 – 102. Continuous flow multistep synthesis. T.F. Jamison*

13:25 – 103. Utilization of microflow technology for the site-selective modification of multifunctionalized molecules. S. Fuse, Y. Mifune, N. Tanabe, H. Nakamura, T. Takahashi

13:40 – 104. Synthesis of diisobutyl aluminum borohydride for the reduction of tertiary amides at ambient temperatures with the potential for continuous flow chemistry. R. Snelling, B. Singaram*

13:55 – 105. Bond expandability of the ultralong C-C bond in unsymmetrically substituted tetraalkylpyracyenes prepared by a flow microreactor method. T. Suzuki*, Y. Uchimura, T. Takeda, R. Katono, H. Kawai, K. Fujiwara, A. Nagaki, J. Yoshida

14:10 – 106. Three-component coupling of benzene based on flash chemistry. T. Kitamura, D. Ichinari, A. Nagaki, J. Yoshida*

14:25 – 107. Microfluidic approach to integrated synthesis of thioquinazolinone derivatives. H. Kim, H. Lee, d. kim*, J. Yoshida*

14:40 – 108. Synthesis and reactions of ynolates using flow microreactors. M. Shindo*

14:55 – 109. Synthesis and application of hexafluoropropyl methyl ether. D. Lokhat*, K. Padayachee, A.K. Domah, N. Sunthapul, N. Seocharan, D. Ramjugernath

15:10 – 110. Highly selective synthesis of organofluorine compounds using flow microreactors. H. Amiti*

15:25 – 111. Generation and reactions of perfluoroalkyl-substituted organolithiums using flow microreactors. K. Hirose, K. Akahori, S. Tokuoka, A. Nagaki, J. Yoshida*

15:40 – 112. Flow carbonylation based on reactive acyl intermediates. I. Ryu*

16:05 – 113. Various applications of bacteriogenic iron oxide in a tube reactor and other systems for organic synthesis. K. Mandai, T. Fukuda, Y. Miyazaki, N. Hanata, H. Mandai, H. Hashimoto, T. Erna, J. Takada, S. Suga*

16:20 – 114. Toward development of chemo-enzymatic reactions under continuous-flow conditions. R.M. de Souza*

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

Molecular and Supramolecular Photochemistry (#71)

Organized by: J. Sivaguru, W. Chung, C. Bohne, c. Tung, M. Sakamoto, V. Ramamurthy
Presiding: S. Jayaraman

13:00 – 115. Self-assembled bis-urea macrocycles as containers for oxidations, polymerizations, and photochemical reactions. L.S. Shimizu*

13:30 – 116. Bright fluorescent nanotags for bioimaging and detection based on bottle-brush polymers with DNA-tipped bristles. B. Armittage*

14:00 – 117. Excited singlet states of firefly light-emitter analogs in luciferase supramolecular environments. T. Hirano*

14:30 Break

14:45 – 118. Molecular recognition and photochemistry: A match made in heaven?. D. Bassani

* Principle Author

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onlineprogram

15:15 – 119. Supramolecular nanocarriers with photoresponsive cargo. **F.M. Raymo**
15:45 Break
16:00 – 120. Charge-transfer band excitations in donor-acceptor systems. **T. Mori**
16:30 – 121. Unique photochemical properties and reactions of clay nanosheet-organic dye complexes. **S. Takagi***, Y. Ishida, T. Shimada, V. Ramamurthy*

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74)

Organized by: R. Danheiser,
T. Fukuyama, M. Lautens
Presiding: T. Fukuyama

13:00 – 122. Synthesis of nakadomarin A and manzamine A from a single advanced intermediate. **J.S. Clark**, C. Xu, G. Meier
13:20 – 123. Total synthesis of dihydrooxepine-containing epidithiodiketopiperazine natural products. **H. Tokuyama***
14:00 – 124. Carbofunctionalization en route to heterocycles. **M. Lautens**
14:40 – 125. Necessity is the mother of invention: Development and application of new methods for the synthesis of alkaloids. **S.E. Reisman**
15:20 – 126. Intramolecular Larock reaction and applications to the synthesis of N-heterocyclic natural products. **Y. Jia**
16:00 – 127. Intramolecular dearomatizing [3+2] annulation of α -imino carbene complexes with aryl rings furnishing 3,4-fused indole skeletons. **T. Miura***, Y. Funakoshi, M. Murakami*
16:20 – 128. Stereoselective functionalizations of alkenes: The power of chiral hypervalent iodine reagents. **T. Wirth***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Homogeneous Gold Catalysis: Methods, Theories and Applications (#192)

Organized by: L. Zhang, H. Ohno, R. Liu
Presiding: L. Zhang

13:00 – 129. Gold/Lewis acid combined catalysis for domino cycloaddition reactions. **Z. Xu***
13:20 – 130. Gold-catalyzed cascade cyclizations of alkynes for construction of nitrogen heterocycles. **H. Ohno***
13:50 – 131. Gold-catalyzed tandem cyclopropanation/Cope rearrangement/C–H activation of dienedynes for the construction of seven-membered ring-containing polycycles. **Z. Yu**
14:10 – 132. Gold-catalyzed cascade reactions. **A.M. Echavarren***
14:45 break
15:00 – 133. Gold-catalyzed synthesis of new spiroacetals. **N. Krause***
15:20 – 134. Gold-catalyzed cycloadditions of alkynes with small molecules with alkynes serving as two- or four-carbon building blocks. **R. Liu**
15:50 – 135. Sustainable gold-catalyzed strategies for complex molecule synthesis. **P. Chan**
16:10 – 136. Gold-catalyzed hydride and nitrene transfer reactions. **F. Gagoz***
16:40 – 137. Construction of medium-sized rings through gold(I)-catalyzed alkyne cyclizations with hollow-shaped phosphine ligands. **T. Iwai**, M. Ueno, H. Okochi, M. Sawamura*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Molecular Function of Natural Products: Advances towards Chemical Biology (#237)

Organized by: M. Ueda, B. Miller, K. Irie, B. Miller, B. Miller, C. Lin, T. Oishi, C. Forsyth, H. Lee
Presiding: K. Irie

13:00 – 138. MPlase (membrane protein integrase), a glycopolymer involved in protein integration into and protein translocation across the cytoplasmic membrane of *E. coli*. **K. Nishiyama***, M. Moser, S. Kusumoto, K. Shimamoto
13:15 – 139. Mechanism of cancer-selective pro-apoptotic effect by acyclic retinoid and structurally related compounds derived from foods. **S. Kojima***, X. Qin

13:30 – 140. Theoretical study on the mutual influence of water and biomolecules. **M. Aida**

13:45 – 141. Fluorine containing C-linked gangliosides GM3 analogs: Synthesis, conformational analysis, and biological activities. **G. Hirai***, M. Kato, K. Onuma, E. Nishizawa, H. Koshino, M. Sodeoka*

14:00 – 142. Unified total synthesis of oxygenated cardenolides. **D. Urabe**, M. Inoue*

14:15 – 143. Synthesis and biological activities of guanidine-containing natural products. **T. Nishikawa***, Y. Nakane, A. Nakazaki, T. Imazu, S. Tokoro, R. Sakakibara, M. Adachi, K. Konoki, M. Yotsu-Yamashita

14:30 – 144. Scopadulcol, a diterpenoid isolated from *Scoparia dulcis* by screening for Wnt signal inhibitors, exhibits TRAIL resistance overcoming activity. R.G. Fuentes, K. Toume, M.A. Arai, S.K. Sadhu, F. Ahmed, M. Ishibashi*

14:45 – 145. Synthetic and biological studies of meayamycins, inhibitors of splicing factor 3B unit 1. **K. Koide***, Y. Gao, U. Basu, R. Bressin, S. Osman

15:00 – 146. Natural products-prompted chemical biology: Phenotypic screening and target identification. **H. Kakeya***

15:20 – 147. Design and synthesis of carbohydrate-based probes for labeling interacting proteins. **C. Lin**

15:40 – 148. Natural products-inspired approach to RNA recognition. **B. Miller***

16:00 – 149. Strategies to create diverse collections of natural products. **S.A. Snyder**

16:30 – 150. Recent progress in the synthesis of complex natural products. **J.L. Wood***

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Frontiers of Chirality in Organic Chemistry (#286)

Organized by: J. Canary, N. Berova, E. Yashima, M. Hyun, T. Shibata, T. Asahi, C. Welch, S. You
Presiding: N. Berova

13:00 Introduction

13:05 – 151. Computation of electronic optical activity from first principles. **J. Autschbach**

13:35 – 152. Application of vibrational and electronic CD in structural analysis of natural products: Reliability assessment on a quantitative level. **A.G. Petrovic***, M. Evidente, N. Berova

13:50 – 153. Chirality sensing with stereodynamic chemosensors. **C. Wolf***

14:05 – 154. Theoretical models for the calculation of resonance Raman optical activity spectra of complex systems. **C. Cappelli**

14:20 – 155. Optimization and validation of the measurement of VCD. **L.A. Nafie***
14:50 Break

15:00 – 156. VCD exciton chirality method: Stereochemical determination of small-, medium- and large-sized molecules without theoretical calculation. **K. Monde***, T. Hongen, D. Manai, T. Taniguchi

15:30 – 157. VCD spectroscopy: A powerful new tool for probing solvent-induced helicity inversion and intermolecular interactions in solution. **Y. Xu***

16:00 – 158. Chiroptical signal enhancement and intrinsic limitations. **M. Cho**, H. Rhee

16:30 – 159. Chiroptical response in porphyrin Soret band region - a powerful and diagnostic structural probe. **N. Berova***, R. Purrello

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Supramolecular Chemistry at the Interface of Materials, Biology, and Medicine (#300)

Organized by: S. Zimmerman, Z. Li, K. Kim
Presiding: Z. Li

13:00 – 160. Applications of cucurbiturils in chemistry, biology, and materials. **K. Kim***

13:30 – 161. From self-assembly to antimicrobial properties: Depolarization and weakening of the bacterial membrane by synthetic anion transporters. **A.R. Schmitz***

14:00 – 162. Development of pseudorotaxane formation methods targeting on nucleic acids. **K. Onizuka***, Y. Ito, H. Abe, F. Nagatsugi

14:20 – 163. Trehalose glycopolymer hydrogels and nanoparticles for stabilization and delivery of proteins. **H. Maynard***, J. Ko, J. Lee

14:50 – 164. Construction of 2D supramolecular polymers through self-assembly: Design, characterization, and properties. **X. Zhao***

15:10 – 165. Sugar-coated polyplexes: Designed glycopolymers for nucleic acid delivery. **T.M. Reineke***

15:40 – 166. Supra-amphiphiles: From molecular architectures and functions. **X. Zhang**

16:10 – 167. Synthesis, recognition properties, and applications of macrocyclic cucurbit[n]urils and their derivatives. **L. Isaacs***

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Nanomaterials as Catalysts for Green Chemistry (#313)

Organized by: A. Moores, Y. Uozumi, C. Li, R. Varma

13:00 – 168. Nanostructured materials for catalytic applications. **J.Y. Ying***

13:20 – 169. Development of a silicon nano-wire array-stabilized palladium nanoparticle catalyst and its application to organic reactions. **Y.M. Yamada***, Y. Yuyama, T. Sato, S. Fujikawa, Y. Uozumi

13:40 – 170. Easy synthesis of metal nanoparticle catalysts for organic reactions under mild conditions. **J. Park***

14:00 – 171. Recyclable “boomerang” linear polystyrene-stabilized Pd nanoparticles for a series of C–C coupling reactions in water. **A. Ohtaka***, E. Sakaguchi, T. Okagaki, G. Hamasaki, Y. Uozumi, O. Shimomura, R. Nomura

14:20 – 172. Phosphine-cross-linked polystyrenes as platforms for producing highly active heterogeneous transition metal catalysts. **M. Sawamura***

14:40 Break

15:00 – 173. Photochemical reactions on plasmonic metal nanostructures. **S. Linic**

15:20 – 174. Redox-selective conversion of alcohols using metal-loaded photocatalysts. **H. Naka***, J. Caner, Z. Liu, Y. Takada, A. Matsuoka, A. Kudo, S. Saito*

15:40 – 175. Defect site control in nanostructured metal oxides toward efficient heterogeneous catalysts. **F. Wang***

16:00 – 176. Tuning the thermodynamic activities of reactive oxygen on dispersed metal clusters for oxidation catalysis. **W. Tu, P. Lachkov, Y. Chin**

16:20 – 177. Enhanced catalysis of alkane-thiolate-self-assembled-monolayer-capped gold nanoparticles towards silane alcoholysis. **K. Isono***, T. Taguchi, K. Ishibashi, H.R. Takaya, M. Nakamura, K. Miki*

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

Mechanochemistry and Solvent-free Synthesis (#322)

Organized by: T. Friscic, E. Juaristi, C. Raston

13:00 – 178. Mechanochemistry and supramolecular catalysis in templated solid-state reactions. **L.R. MacGillivray***

13:25 – 179. Grinding assisted metal free organic transformations. **S.S. Chimni***

13:50 – 180. Recent advances in mechanochemical organic synthesis. **G. Wang**

14:15 – 181. (Dis)Advantages of mechanochemical methods in the discovery of novel organic materials. **D. Bucar***

14:35 – 182. Don't throw it away, recycle for another day: The development of recyclable reactions under mechanochemical conditions. **J. Mack***, L. Chen, K. Leahy, R.A. Haley

15:00 – 183. Mechanochemical, solvent-free synthesis of metal and metal sulfide nanoparticles. **A. Moores***, M.J. Rak, T. Friscic, T. Bastalle

15:20 Coffee Break

15:30 – 184. Mechanochemical ligand exchange to control the surface properties of superparamagnetic iron oxide nanoparticles. **A.S. Blum***, K.V. Korpany, J. Bachelder, P. Dong, S. Trudel, C. Mottillo, T. Friscic

15:50 – 185. Explorations of mechanochemical Friedel-Crafts acylations. **M. Djud, V. Strukil, D. Margetic***

16:15 – 186. Fundamental studies of extrusion and other novel approaches to mechanochemical synthesis. **D.E. Crawford***, J. Casabán, N. Girí, R. Haydon, T. McNally, A. Michalchuk, L. Wright, A. Abbott, C. Pulham, S. James

16:35 – 187. Mechanochemistry as an excellent and clean approach for chemical synthesis and discovery. **T. Friscic**

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Carbenes and Carbenoids in Organic Synthesis (#362)

Organized by: K. Scheidt, M. Murakami, R. Chi

13:00 – 188. Catalytic synthesis with azavinyl carbenes. **V. Folkin**

13:25 – 189. Toward carbene organocatalyst-enabled new activation modes. **Y. Chi**

13:50 – 190. Carbene-catalyzed asymmetric benzoin cyclization: Total synthesis of highly oxygenated natural products derived from polyketide-II biosynthesis. **K. Suzuki***, H. Takikawa

14:15 – 191. N-heterocyclic carbene catalyzed carbon–carbon and carbon–heteroatom bond formation via vinyllogous enolates and allenolates. **J. Sun***

14:40 PM Break

15:00 – 192. Intramolecular formal C–H insertion reaction of photochemically-generated siloxycarbenes leading to benzofused heterocycles. **T. Nakada, S. Ishii, K. Ishida, N. Iwasawa, H. Kusama***

* Principle Author

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15:25 – 193. Cross-coupling reactions through migratory insertion of metal carbene. **J. Wang**
15:50 – 194. New planar chiral cabenes for catalysis. **K. Scheidt**
16:15 – 195. Reactions of alpha-imino metal carbene complexes generated from *N*-sulfonyl-1,2,3-triazoles with sulfur compounds. **M. Murakami**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Cognizance of Endangered Elements for Organic Synthesis (#415)

Organized by: H. Tsuji, S. Zhu,
G. Konishi, C. Luscombe, L. Campeau
Presiding: L. Ilies, H. Tsuji

13:00 – 196. Base metal catalysis an enabling tool for organic chemistry. **P.J. Chirik**

13:30 – 197. Copper or iron-catalyzed organic reactions involving hydrogen transfer processes. **S. Zhu***

14:00 – 198. Iron-catalyzed hydro- and carbometalation of alkynes. **L. Ilies***, T. Yoshida, E. Nakamura*

14:20 – 199. Synthesis, structure, and reactivity of aryliron intermediates in iron-catalyzed cross-coupling reaction.

S. Nakajima, K. Isozaki, N. Nakagawa, R. Imayoshi, T. Hashimoto, N.J. Gower, L. Adak, T. Honma, M. Takagaki, Y. Sunada, H. Nagashima, D. Hashizume, O. Takahashi, T. Iwamoto, T. Hatakeyama, H.R. Takaya*, M. Nakamura*

14:40 Break

14:55 – 200. Searching for new reactivity: Iron-catalyzed stereoselective olefin aminohydroxylation and aminofluorination reactions. **H. Xu**

15:25 – 201. Hydrosilylation of alkenes by common metal catalyst systems. **H. Nagashima***, D. Noda, Y. Sunada, A. Tahara

15:55 – 202. Molybdenum-catalyzed stereospecific deoxygenation of epoxides. **S. Asako***, T. Sakae, T. Nakagiri, K. Takai*

16:15 – 203. Catalyst design of Vaska-type iridium complexes for efficient synthesis of π -conjugated enaminones. **A. Tahara**, Y. Sunada, Y. Motoyama, H. Nagashima*

Wednesday Morning

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Reactive Intermediates and Unusual Molecules (#7)

Organized by: R. Sheridan, M. Abe, W. Leigh

8:00 – 204. Benzoin condensation and related reactions: Gas phase experimental and computational studies. **Y. Tian**, Y. Niu, J.K. Lee*

8:25 – 205. Experimental studies of quinonimides and benzaldimides. **P. Wentholt***

8:50 – 206. Falling solid flash vacuum pyrolysis. **C. Wentrup***

9:15 – 207. Controlling the selectivity of photo-Michael “click” reaction with pH. **V. Popik**

9:40 – 208. Bimolecular reactions of silicon (Si) and silylidene (SiH) with small unsaturated hydrocarbon molecules. **T. Yang***, B. Dangi, P. Maksyutenko, R. Kaiser, L. Bertels, M. Head-Gordon

10:00 – 209. New materials for singlet fission. **J. Wen**, S. Nedungadi, A. Younes, J. Kaleta, J. Plutnar, Z. Havlas, J. Johnson, J. Michi*

10:25 – 210. Cage-type radical cations with the nature of “One-Electron C–C σ Bond”. **H. Ikeda***

10:50 – 211. Interfacial photochemistry for materials modification. **M. Workentin**, P. Gobbo, W. Luo, V. Popik, D. Sutton, C. McNitt

11:15 – 212. Synthesis and properties of a stable germbenzenylpotassium. **N. Tokitoh***, S. Fujimori, Y. Mizuhata, T. Sasamori
11:40 – 213. Direct detection of transient stannylenes in solution by laser flash photolysis. **W.J. Leigh***, I.R. Duffy

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

Prospects for Flow Chemistry (#29)

Organized by: J. Yoshida, T. Jamison, D. Kim, M. Organ
Presiding: A.A. Kulkarni, M.G. Organ

8:00 – 214. New advances in flow chemistry. **D. Mallik**, M. Tilley, G. Li, A. Khadra, K. Somerville, M. McGuire, **M.G. Organ**

8:25 – 215. Solid phase catalyst confined in multiwalled carbon nanotubes: Catalytic asymmetric nitroaldol and Mannich-type reactions in a continuous-flow platform. **N. Kumagai***, K. Hashimoto, M. Shibusaki*

8:40 – 216. Heterogeneous metal nanoparticle catalysts for multiphase flow processes. **H. Miyamura**, S. Kobayashi*

8:55 – 217. Selective transformation of alkynes with nanoporous gold catalyst. **Y. Ishikawa**, T. Jin, Y. Yamamoto, N. Asao*

9:10 – 218. Dual role flow reaction system containing an amphiphilic polymer-dispersion of platinum nanoparticles for oxidation and reduction. **T. Osako**, K. Torii, A. Tazawa, Y. Uozumi*

9:25 – 219. Microfluidics and carbon dioxide. **E. Kumacheva**

9:50 – 220. Intensification of flow ATRP polymer syntheses by microreaction technologies. **D. Parida**, **C.A. Serra***, D.K. Garg, Y. Hoarau

10:15 – 221. Multistep flow synthesis: Synchronizing the synthesis and work-up time scales. **A.A. Kulkarni***, Y. Sharma, M. Sharma, R.A. Joshi

10:40 – 222. Precision polymer synthesis in continuous microflow: Challenges and perspectives. **T. Junkers***

10:55 – 223. Synthesis of multifunctional polymers by RAFT method and droplet microfluidic approach for cancer cells imaging. **L. Qi***

11:10 – 224. On the generation of butyl rubber in a microflow device. **Y. Lu***, S. Zhu, K. Wang, G. Luo

11:25 – 225. Rhodium-catalyzed arylation of vinyl ethers with Grignard reagents and its mechanistic studies using a flow micro reactor. **T. Iwasaki**, R. Akimoto, Y. Miyata, H. Kuniyasu, N. Kanbe

11:40 – 226. Direct manipulation of particle size and morphology of ordered mesoporous silica by flow synthesis. **K. Yeung**

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

Molecular and Supramolecular Photochemistry (#71)

Organized by: J. Sivaguru, W. Chung, C. Bohne, c. Tung, M. Sakamoto, V. Ramamurthy
Presiding: C. Bohne

8:00 Zimmerman symposium Remarks

8:05 – 227. One and two photon release of new bioactive initiators/substrates from ρ -hydroxyphenacyl cages. **R.S. Givens***

8:35 – 228. Photochemical cyclizations of enynes and endineynes: Optimizing electronic and stereoelectronic factors. **I. Alabugin***, R. Mohamed

9:05 – 229. Development of photolabile protecting groups. **P. Wang**

9:35 Break

9:50 – 230. Topological activation of fluorophores for imaging and sensors. **L.M. Tolbert***, K. Solntsev

10:20 – 231. Photochemistry and spectroscopy of thiophene carbenes. **R.J. McMahon***, C.R. Pharr, L.A. Kopff

10:50 Break

11:05 – 232. Intramolecular cycloadditions of photogenerated azaxylenes and quinomethanes. **A.G. Kutateladze***, O.A. Mukhina, N. Kumar

11:35 – 233. Decarboxylative radical reactions of aliphatic carboxylic acids via photoinduced electron transfer. **Y. Yoshimi**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74)

Organized by: R. Danheiser, T. Fukuyama, M. Lautens
Presiding: M. Lautens

8:00 – 234. Photoassisted synthesis of complex nitrogen polyheterocycles. **A.G. Kutateladze***, O.A. Mukhina, N. Kumar, W.C. Cronk, W.J. Umstead, D.M. Kuznetsov

8:20 – 235. New methods for the construction of biologically relevant nitrogen heterocycles. **M.G. Banwell***

9:00 – 236. New cycloaddition strategies based on strained and unusual molecules. **R. Danheiser***

9:40 – 237. New methods for N-C bond formation. **P.S. Baran**

10:20 – 238. New annulative routes to heterocycles from donor-acceptor cyclopropanes. **M.A. Kerr**

11:00 – 239. Aiming divergent syntheses of polycyclic natural products. **J. Shimokawa***, M. Kitamura*, T. Fukuyama*

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Practical Application of Basic Research on Molecular Recognition (#136)

Organized by: C. Tran, K. Kano, C. Easton
Presiding: C.D. Tran, M.W. Urban

8:00 Opening Remarks

8:05 – 240. Tunable solid-state fluorescent materials for supramolecular encryption. **J.F. Stoddart***, X. Hou, C. Ke

8:30 – 241. Evolution of chiral recognition and separations: New selectors and ultra-fast analyses. **D.W. Armstrong***

8:55 – 242. From stimuli-responsive polymers to self-repairing materials. **M.W. Urban***

9:20 Break

10:00 – 243. Differential sensing, theory, and applications. **E.V. Anslyn***

10:25 – 244. Molecular fibres and wires in solid-state and solution self-assemblies of cyclodextrin [2]-rotaxanes. **C.J. Easton***

10:50 – 245. Chemical tools to isolate a desired fragment from human genome. **M. Komiyama**

11:15 – 246. Analyses for recognition function of glycolipids using planar lipid membranes. **T. Sato**

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Homogeneous Gold Catalysis: Methods, Theories and Applications (#192)

Organized by: L. Zhang, H. Ohno, R. Liu
Presiding: R. Liu

8:00 – 247. Gold and copper-catalyzed skeletal rearrangement of O-propargylic oximes. **I. Nakamura***, S. Gima, Y. Kudo, M. Terada

8:20 – 248. Selectivity control in gold-catalyzed reactions. **J. Zhang**

8:50 – 249. Selective synthesis of complex carbocycles via a one-pot gold(I)-catalyzed cyclization. **L. Barriault**, G. Revol, F. Barabé, P. Levesque

9:10 – 250. Reactivity driven discovery of gold-catalyzed reaction for organic synthesis. **F. Toste**

9:45 break

10:00 – 251. One-pot synthesis of enantio-enriched fluorinated cyclopentenones and 4,9-dihydro-1*H*-carbazoles by the combination of gold catalysis and asymmetric Lewis acid catalysis. **L. Ye***, A. Zhou

10:20 – 252. Gold and its combination with chiral Brønsted acids for asymmetric catalysis. **L. Gong***

10:50 – 253. Gold-catalyzed post-Ugi heteroannulations and domino reactions. **E. Van der Eycken***

11:10 – 254. Gold-catalyzed enantioselective synthesis of azahelicenes. **K. Tanaka***

11:40 – 255. Reinventing cycloaromatization reactions with Au-catalysis: Switch from diradical to zwitterionic pathways. **I. Alabugin**, G. dos Passos Gomes

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Molecular Function of Natural Products: Advances towards Chemical Biology (#237)

Organized by: M. Ueda, B. Miller, K. Irie, B. Miller, B. Miller, C. Lin, T. Oishi, C. Forsyth, H. Lee
Presiding: C. Forsyth

8:00 – 256. Mechanistic evaluation of the inhibition of polycyclic mutagens by endogenous bile pigments. **J.T. Blanchfield***, H.T. Hung, A. Bulmer, K. Wagner, J. De Voss, A. Abu Bakar

8:15 – 257. Nitrimine coupling reactions in the synthesis of biologically active molecules. **V.V. Angeles-Dunham**, A.E. Mattson*

8:30 – 258. Tyrosine-selective chemical modification using single-electron-transfer catalyst. **S. Sato**, K. Nakamura, H. Nakamura*

8:45 – 259. One-pot sequential palladium-catalyzed cross-coupling reaction of cyclic boron compounds. **R. Suzuki**, K. Sato, S. Fuse, **H. Tanaka**

9:00 – 260. Studies on synthesis and structure-activity relationships of neuroactive glutamate analogs. **M. Oikawa**, M. Chiba, K. Fukushima, K. Kawamura, Y. Ishikawa

9:30 – 261. Development of artificial assembly line for skeletally diverse natural products and its variants. **H. Oguri***

10:00 – 262. New directions in the Fischer indole synthesis. **C. Cho***

10:30 – 263. Structure-activity relationship studies of maitotoxin based on chemical synthesis of partial structures. **T. Oishi***

11:00 – 264. Privileged structures as efficient chemical navigators toward unexplored biologically relevant chemical spaces. **S. Park***

11:30 – 265. Discovery, characterization, and synthesis of natural products with activity against Gram-negative pathogens. **J.B. MacMillan***

* Principle Author

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Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Frontiers of Chirality in Organic Chemistry (#286)

Organized by: J. Canary, N. Berova, E. Yashima, M. Hyun, T. Shibata, T. Asahi, C. Welch, S. You
Presiding: M. Hyun

8:00 Introduction

8:05 – 266. Synthesis and enantioseparation ability of immobilized polysaccharide-based chiral stationary phases for HPLC. **Y. Okamoto**

8:35 – 267. Development of crown ether-based chiral stationary phases based on (+)-(18-crown-6)-2,3,11,12-tetracarboxylic acid and their applications. **M. Hyun***

9:05 – 268. Recent applications of chiral chromatography for pharmaceutical discovery and development. **C. Welch**

9:35 – 269. Controlled synthesis and chiral recognition ability of polysaccharide derivatives bearing regioselective substituents. **J. Shen**

10:05 Break

10:15 – 270. Endogenous D-amino acids in the nervous and endocrine systems: From formation and release to function. **S.S. Rubakhin, A.V. Patel, N. Ota, J.V. Sweedler**

10:30 – 271. Ultrafast chiral separations: Praxis, performance, and peculiarities. **D.W. Armstrong***

11:00 – 272. Pushing the speed limits in chiral supercritical fluid chromatography. **E.L. Regalado***

11:15 – 273. Supramolecular methods for the rapid determination of enantiomeric excess. **E.V. Anslyn**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Supramolecular Chemistry at the Interface of Materials, Biology, and Medicine (#300)

Organized by: S. Zimmerman, Z. Li, K. Kim
Presiding: S. Zimmerman

8:00 – 274. Helical aromatic amide foldamers: Some new advances. **Z. Li***

8:30 – 275. Triptycene-derived macrocyclic hosts for molecular recognition and self-assembly. **C. Chen**

9:00 – 276. Helical polymers and oligomers as unique chiral materials. **E. Yashima**

9:30 – 277. New materials from the supramolecular assembly of cellulose nanocrystals. **M. MacLachlan**

10:00 – 278. Fluorescent RNA labeling using self-alkylating ribozymes. **J. Heemstra**

10:20 – 279. Application of self-assembled nanostructures to organic electronic devices. **J. Hong***

10:50 – 280. One-pot synthesis and self-assembly of P3HT-containing block copolymers. **Z. Wu, N. Liu**

11:10 – 281. Conjugated radical cation dimerization (CRCD) as noncovalent driving force for supramolecular self-assembly. **D. Zhang*, L. Chen, Y. Zhang, J. Tian, L. Zhang, W. Wang, H. Wang, Z. Li**

11:30 – 282. Correlation of molecular properties and supramolecular morphology of cationic lipoplexes with transfection efficiency. **P. Parviz, L. Radu, N. Abdul Khalique, E. Jubeli, D. Nicholson, H. Larsen, M. Pungente, T. Fyles**

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Nanomaterials as Catalysts for Green Chemistry (#313)

Organized by: A. Moores, Y. Uozumi, C. Li, R. Varma

8:00 Break

8:40 – 283. Cellulose nanocrystals as catalysts supports and chiral inducers. **A. Moores, M. Kaushik, C. Cirtiu, C. Benoit**

9:00 – 284. Unsupported palladium nanoparticles for mono- and bi-phasic hydrogenation and redox isomerization of alkenes in water: Structurally stable and reusable micelle catalysts. **M.S. Manung, T. Dinh, Y. Shon***

9:20 – 285. Naked iron and cobalt: The case of homogeneous vs. heterogeneous. **A. Jacob von Wangelin***

9:40 Break

10:00 – 286. Polymer-incarcerated metals: Highly reactive, recoverable, and multifunctional nanoparticle catalysts for green sustainable chemistry. **S. Kobayashi**

10:20 – 287. Mag(net)ic catalysts - synthesis and applications. **O. Reiser***

10:40 – 288. Development of dinuclear copper complex catalyst using interlayer nanospace of magadite for efficient bond formation reactions. **Z. Maeno, T. Mitsuodome, T. Mizugaki, K. Jitsukawa, K. Goto, I. Shibata**

11:00 – 289. Hyperbranched polystyrenes bearing ammonium salts as the support of nanometal particles: Applications to bi-phasic catalyst systems. **H. Nagashima*, L. Gao, K. Kojima**

11:20 – 290. Engineering the catalyst performance of bimetallic nanoparticles for glycerol upgrading. **Z. Zhao*, R. Gonzalez, J. Miller, M.S. Wong**

Hawaii Convention Center
Halls I, II, III

Mechanochemistry and Solvent-free Synthesis (#322)

Organized by: T. Friscic, E. Juaristi, C. Raston

Poster Session

10:00 – 12:00

291. Mechanochemistry: Fundamental questions and commercialisation. **S. James***

292. Solvent-free solid-phase direct reduction of benzaldehydes to benzyl alcohols. **Y. Mitoma*, Y. Matsumoto, N. Egashira, C. Simion, M. Tanaka**

293. Mechanochemistry as a tool for reaction discovery: New copper catalyzed mechanochemical C-N coupling reactions. **D. Tan, T. Friscic**

294. Thermal effects in mechanochemical milling reactions. **K. Uzarevic, I. Halasz, C. Mottillo, P. Julian, A. Puskaric, V. Strukil, T. Friscic***

295. Mechanochemieal synthesis of MOF-74 family of metal-organic frameworks. **K. Uzarevic, P. Julian, A. Katsenis, I. Halasz, T. Friscic***

296. Templation effects and novel ZIF structures by solid state synthesis. **I. Brekalo*, J.R. Ramirez, C.M. Kane, K.T. Holman**

297. Mechanochemical synthesis of a series of meso-tetrasubstituted porphyrins. **Q. Su, T. Hamilton***

298. Atom economic and environmentally benign synthesis of oxindoles by metal-catalyzed cyclization under solvent-free and aerobic condition. **H. Shin, S. Kim, W. Lee*, J. Choi, H. Ha***

299. JEDI analysis of the distribution of mechanical stress in polymer knots. **T. Stauch*, A. Drew**

300. Mechanochemistry as a greener route to biological porphyrin targets. **D. Cordero, T. Hamilton***

301. Mechanochemistry for the green preparation of bioactive hydantoins. **E. Colacicino***

302. Ball-milling as solventless green technology for revisiting the N- and C-protection of amino acids and esters. **E. Colacicino***

303. Solvent-free mechanochemical synthesis of hierarchical ZIF-8 MOF. **S. Tanaka, A. Yasuyoshi, Y. Miyake, G.V. Baron, J.F. Denayer**

304. Development of the new versatile reaction field for various organic reactions. **M. Ohmura, Y. Ishimura, Y. Ikeda, S. Kamino, D. Sawada***

305. Effect of high pressure on the Raman spectra of some solid mechanochemically-produced halogen-bonded Co-crystals. **I.S. Butler*, Y. Desjardins-Langlais, J. Poisson, C. Nickels, T. Friscic**

Hawaii Convention Center
Halls I, II, III

Carbenes and Carbenoids in Organic Synthesis (#362)

Organized by: K. Scheidt, M. Murakami, R. Chi

Poster Session

10:00 – 12:00

306. Ring-expansion reaction of vinylsulfonium ylides generated by the reaction of vinylcarbenoids with 2-aryl-1,3-dithiolanes. **T. Koizumi*, Y. Ichinose, K. Oshima, Y. Nakata, H. Takahashi, K. Goto, I. Shibata**

307. Ruthenium-catalyzed cycloisomerization of alkynes containing a heterocatom-heteroatom bond: From repulsive to resonance interactions. **S. Roh*, I. Kim, S. Kim, C. Kim, C. Lee***

308. Highly enantioselective synthesis of cyclopropane ring fused γ -lactones via intramolecular carbene transfer reactions. **Y. Nakagawa*, S. Chanthamath, N. Nakayama, H. Goto, K. Shibatomi, S. Iwasa**

309. Highly enantioselective C–H insertion reaction of N-alkyldiazoacetamides by using Ru(II)-phenoxy complex. **T. Doan Thi, S. Chanthamath, K. Shibatomi, S. Iwasa***

310. Carbohydrate-based N-heterocyclic carbenes (NHCs) for asymmetric catalysis. **A.S. Henderson*, J. Bower, M. Galan***

311. Ionic liquids as precatalysts in the highly stereoselective synthesis of 1,6-ketoesters. **L. Ta, A. Axelsson, J. Bjil, H. Sundén***

312. Kinetic study on rhodium(II)-catalyzed cyclopropanation of sulfonyl-1,2,3-triazoles. **S. Kwok, V. Fokin***

313. Ruthenium porphyrin catalyzed three-component reaction for the synthesis of multifunctionalized isoazolidines and aziridines. **A. Reddy, C. Zhou, C. Che**

314. Asymmetric synthesis in green solvents: Homoenolate reactions of N-heterocyclic carbenes. **J.J. Kiddle, D. Kidd**

315. Regioselective functionalization of 1,4-dicarbonyls through the rhodium(II)-carbenoid promoted sigma-motropic rearrangement. **J. Lee, D. Jung, S. Lee***

316. Synthetic study of thermalcalconane B using NHC-catalysis. **Y. Kitahara, A. Tsunoi, T. Utsunomiya, K. Tazawa, K. Manabe, Y. Suzuki**

317. Total synthesis of (+)-tanikolide and its analogs by traceless stereoinduction method using Rh(II)-catalyzed oxonium ylide formation –[2,3]-sigmatropic rearrangement. **H. Jinnochi, H. Nambu, T. Fujiwara, T. Yakura**

318. Tandem rhodium/Lewis acid-catalyzed reaction of N-sulfonyl-1,2,3-triazoles and 2,3-epoxy alcohol: A new route to oxa-zine derivatives. **Y. Ko, S. Lee***

319. Catalyst design for chemoselectivity in the NHC-catalyzed cross-benzoin reaction. **S. Langdon, C.Y. Legault, M. Gravel***

320. Robust pocket recognizing the chirality of amines and showing chiral switching in acetone. **Y. Jin*, Y. Choi, S. Park, K. Kim**

321. Highly stereoselective cyclopropanations of Weinreb amide derivatives using novel Ru(II)-phenoxy catalysts. **H.S. Mandour, S. Chanthamath, K. Shibatomi, S. Iwasa***

322. Stereoselective synthesis of α,β -disubstituted γ -lactones promoted by binaphthyl Ru-carboxylate catalyst. **W. Lu, P. Xu, T. Furuta*, T. Kawabata**

323. N-heterocyclic carbenes for nucleophilic acylation. **K. Dobashi, Y. Suzuki, e. ishitubo, H. Tokiwa**

324. Ru(II)-Phenoxy catalyzed carbene transfer reactions of diethyldiazoethylphosphonate. **S. Ozaki, S. Iwasa*, S. Chanthamath, K. Shibatomi**

325. Enantio- and diastereoselective intra-molecular C–H insertion of α -diazoesters catalyzed by chiral dirhodium(II) carboxylates. **T. Miyazawa, K. Minami, K. Imai, K. Takeda, M. Anada, S. Matsunaga, S. Hashimoto***

326. Synthesis of planar chiral [2.2]paracyclophane-based bisoxazoline ligands bearing no central chirality and application to Cu-catalyzed asymmetric O–H insertion reaction. **s. kitagaki*, K. Sugisaka, K. Asaka, S. Murata, N. Takenaga, C. Mukai**

327. Exploration of an ester alternative and application as a pronucleophile for direct catalytic asymmetric Mannich reaction catalyzed by *N*-heterocyclic carbene. **A. Takahashi*, S. Handa, H. Sugimoto***

328. Synthesis and characterization of multi-nuclear Au complexes bridged by two 1,2,3-triazolylidene carbene-phosphine hybrid ligands. **M. Nishimura, K. Amaike, T. Ooi*, K. Itami*, K. Ohmatsu, J. Yamaguchi**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Cognizance of Endangered Elements for Organic Synthesis (#415)

Organized by: H. Tsuiji, S. Zhu, G. Konishi, C. Luscombe, L. Campeau

Presiding: G. Konishi, C. Luscombe

8:00 – 329. Potential of carbon: Can it be an alternative to rare and precious elements? **H. Tsuiji***

8:20 – 330. Pyrene-based D– π –A dyes with pyridyl carboxamide substituent as a novel acceptor exhibit high quantum yield and perfect solvatochromic fluorescence in apolar and polar solvents. **C. Chen, G. Konishi**

8:40 – 331. Bright and colour-tunable aggregation induced emission of sterically congested D– π –D quadrupolar dyes and their excited-state dynamics. **S. Sasaki*, G. Konishi**

9:00 – 332. Molecular recognition of doubly phosphorus-containing molecular host. **M. Yamamura, T. Nabeshima**

9:20 – 333. Triplet-energy control of PAHs by heteroatom incorporation for development of OLED materials. **T. Hatakeyama*, T. Ikuta, K. Shirien, S. Hashimoto, S. Nakatsuka, H. Hirai, K. Nakajima, J. Ni, M. Nakamura**

9:40 Break

9:55 – 334. Short syntheses of polycyclic aromatic hydrocarbons by catalytic arylation of C–H and C–O bonds in aromatic ketones. **F. Kakuchi**

10:25 – 335. Facile synthesis of ethene-bridged terthiophenes and their physical properties. **K. Mitsudo*, H. Sato, J. Goto, A. Yamasaki, S. Suga***

10:45 – 336. Facile synthesis of fluorene-based conjugated polymers via direct arylation polycondensation. **T. Kanbara*, H. Saito, J. Kuwabara**

11:15 Closing Remarks

* Principle Author

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Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

Photoredox Catalysis in Organic Synthesis (#440)

Organized by: D. Nicewicz, S. Fukuzumi, W. Xiao
Presiding: D. Nicewicz

8:00 Opening Remarks

8:05 – 337. Enantioselective photochemistry via tandem photoredox and Lewis acid catalysis. **T.P. Yoon***

8:40 – 338. Controlled perfluoroalkylation of alkynes and alkenes. **E. Cho***

9:10 – 339. Proton-coupled electron transfer in organic synthesis and asymmetric catalysis. **R.R. Knowles**

9:30 – 340. Regioselective difunctionalization of olefins by photoredox catalysis. **T. Koike***, M. Akita

10:00 Break

10:15 – 341. Synthetic control of photoinduced electron transfer of cyclometalated Ir(III) and Pt(II) complexes and applications to photoredox catalysis. **Y. You***

10:45 – 342. Photoinduced electron transfer mechanism for β -carbonyl Mannich functionalization. **J. Jeffrey***

11:05 – 343. Photoredox catalysis for azide anion activation. **A.G. Griesbeck**

11:25 – 344. Visible light mediated free radical chemistry. **C. Stephenson**

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

Catalytic Multicomponent, Tandem and Cascade Reactions (#445)

Organized by: B. Arndtsen, J. Montgomery, K. Nozaki
Presiding: B. Arndtsen, J. Montgomery, K. Nozaki

8:00 – 345. Chain walking as a strategy for catalytic organic synthesis. **T. Kochi***

8:30 – 346. Alkyl-alkyl bond formation by cascade cyclization-coupling reactions catalyzed by first-row transition metal complexes. **D.J. Cárdenas***, M.E. Bujuel, M. Guisán-Ceinos, F. Tato, R. Soler-Yanes, D. Collado

8:50 – 347. Cascade reactions enabled by nickel and copper catalysis. **J. Montgomery***

9:20 – 348. Diversity-oriented asymmetric catalysis (DOAC) for spirooxindoles. **T. Arai**

9:40 – 349. Sequential catalysis via the combination of Ru/chiral phosphoric acid. **S. You**

10:10 Break

10:20 – 350. Multistep, multicatalytic processes for organic synthesis. **J.F. Hartwig**

10:50 – 351. Tandem applications of process analytical technology to accelerate reaction discovery and optimization. **J. Hein**

11:10 – 352. Bifunctional acid-base mixed oxide catalysts for cascade reactions in ethanol conversions. **K. Ramasamy***, c. Smith, M. Gray, H. Job, y. wang

Hawaii Convention Center
Halls I, II, III

Organic General Posters
10:00 – 12:00

Asymmetric Synthesis

353. Synthesis of tetracyanocyclopentadienide salts featuring a chiral BINOL auxiliary. **J. Matsuoka**, T. Sakai*, Y. Mori*

354. Hydrolysis and stereococonversion of amino acid esters by ARCA and its reaction mechanism. K. chun, **T. Kim**

355. Enantioselective 1,2-addition of aryl Grignard reagents to ketones. **K. Osakama**, M. Nakajima*

356. Chiral N -(*tert*-butyl)- N -methylaniline type ligands: Synthesis and application to palladium-catalyzed asymmetric allylic alkylation. **T. Mino***, M. Asakawa, Y. Shima, M. Sakamoto

357. Catalytic enantioselective amidation of α -amino acid derivatives by a chiral *tert*-amine catalyst. **K. Masaki**, M. Kitamura, S. Sasaki, M. Kunishima*

358. Chiral lithium binaphtholate catalyzed enantioselective Michael additions of acyclic α -alkyl- β -keto esters. **M. Moritani**, S. Kotani*, M. Nakajima

359. Synthesis and structure of macrocyclic pybox complexes. **S. Komagawa**, T. Huke, M. Ueno, K. Yamaguchi*

360. Enantioselective α -arylation of esters: Redesign of a ligand to solve a classical synthetic challenge. **P. Zhang**

361. Axially chiral biaryl dials: A chiral shift reagent for primary amines. **S. Kim**, G. Lee, S. Lee, H. Han

362. Highly regio- and enantioselective hydrostannation of alkynes. **J. Park**, S. Gupta, Y. Do, J. Lee, M. Lee, J. Han, Y. Rhee*, J. Park*

363. Regiochemistry-directed syntheses of polyhydroxylated alkaloids from chiral aziridine. **J. Choi**, H. Eum*, H. Ha, C. Cho

364. Highly regio- and stereoselective ring expansion of chiral aziridines: Application toward the asymmetric synthesis of nitrogen containing heterocycles. **J. Choi**, N.Y. Yadav, H. Ha

365. Enantio- and diastereoselective conjugate addition of 1-pyrroline 5-carboxylate esters to nitroalkenes catalyzed by silver and copper complexes with chiral ferrocenyl ligands. **M. Kimura***

366. Asymmetric Favorskii rearrangement of α -chloro- β -keto esters. **N. Sasaki**, M. Kotozaki, K. Shibatomi*, S. Iwasa

367. Investigation of *tert*-butylsulfurylmethyl substituted aryl compounds for stereocontrolled condensation with an electrophile. **J. Wei**, Z. Sun*

368. Optical resolution of 1,2-diphenylethylene diamine using diastereomeric salt formation method. **S. Kishimoto**, T. Kijima, W. Fujiwara, S. Murakami, S. Matsuba, B. Hatano

369. Stereoselective synthesis of 3-hydroxy-4-aryl cyclopentanones through a Heck-Matsuda desymmetrization. **R.C. Carmona***, C.D. Correa

Catalysis
370. Formation of cyclic carbonates from CO₂ and epoxides catalyzed by a new type of Lewis acid-base bifunctional M(salphen) (M=Zn, Cu and Ni). **Y. Ren***, H. Jiang*

371. Synthesis of cyclopentadienyl rhodium complexes bearing a cyclodextrin and their application to catalytic reactions. **H. Yamauchi**, S. TSUDA, T. Iwasaki, S. Fujiwara, H. Kuniyasu, N. Kambe

372. Imidazopyridine-palladium catalyzed Mizoroki-Heck reaction. **N. Koza**, F. Yagishita*, K. Nomura, T. Mino, Y. Kawamura, M. Sakamoto

373. Indium-catalyzed formal N-arylation and N-alkylation of pyroles with amines. **K. Yonekura**, O. Kenji, T. Tsuchimot

374. Rhenium-catalyzed isomerization of *N*-alkylpropargylamines to *N*-alkylidenearylamines. **Y. Fukumoto***, **N. Okazaki**, N. Chatani

375. Pd-catalyzed asymmetric intermolecular hydroalkoxylation of alkoxylalene. **S. Kang**, J. Lee, K. Seo, Y. Rhee*

376. Nickel-catalyzed stannylation of organohalides. **K. Komeyama***

377. Mn-catalyzed alkyl-Heck-type reaction via oxidative decarbonylation of aldehydes. **Z. Zong**

378. Transition metal-catalyzed oxygenative α -addition and β -alkylation of terminal alkynes. **H. Yun**, H. UM, C. Lee*

379. Tris(pentafluorophenyl)borane-catalyzed organofunctionalization of various materials with derivatized-poly(methylhydrosiloxanes). **Y. Masui**, S. Ichii, K. Iwada, K. Kanamori, T. Kamei, K. Nakanishi*, T. Shimada*

380. Rhodium-catalyzed reaction of terminal alkynes with *t*-butylhydrazine leading to nitriles. **Y. Tamura**, Y. Fukumoto*, N. Chatani

381. Nickel-catalyzed reaction of perfluoroarenes with 1,3-butadiene through dimerization of 1,3-butadiene. **X. Min**, T. Iwasaki, H. Kuniyasu, N. Kambe*

382. Mechanistic studies on the organic reactions catalyzed by Pd-Fe₃O₄ heterodimeric nanoparticles. **S. Byun***, B. Kim*

383. Synthesis of anilines from aryl halides via copper-catalyzed amination in aqueous ammonia. **Y. Cho**, H. Jung, H. Jeon*

384. Synthesis and applications of electron deficient triazinephosphine ligands. **K. Abe**, M. Kitamura, M. Kunishima*

385. Cu-catalyzed hydro- and alkylperfluoroarylation of 1,3-butadiene. **K. Okamoto**, T. Iwasaki, H. Kuniyasu, N. Kambe*

386. Rhodium-catalyzed tandem addition-cyclization of alkynyl imines. **K. Choi**, J. Joo*, C. Lee*

387. Direct catalytic conversion of ammonia and allylic alcohols to primary allylamines at room temperature. **R. Shibuya**, L. Lin, T. Ohshima

388. Selective role of zeolites in the electrophilic substitution reactions. **M.H. alotaibi***, K. Smith, G. El-Hiti

389. One-pot preparation of α -aminonitriles by indium-catalyzed three-component coupling reaction of alkynes, amines, and trimethylsilyl cyanide. **Y. Hamachi**, Y. Ogiwara, N. Sakai

390. Direct condensation between phthalide and primary amine in the presence of literally catalytic amount of the Lewis acid catalyst. **I. Takahashi**, S. Hosoi

391. Mechanistic study on the generation of carbon monoxide from phenyl formate and its application to the development of Pd-catalyzed carbonylation at room temperature. **H. Konishi**, M. Matsubara, K. Mori, Y. Ishikawa, H. Hashimoto, H. Tokiwa, K. Manabe*

392. BiCMAP-rhodium catalyzed 1,4-addition of arylboronic acids to coumarin derivatives. **K. Watabane**, T. Mino*, K. Miura, Y. Mizutani, M. Sakamoto

393. Transition metal catalyzed allylation of trifluorotoluene derivatives using allylsilane. **T. Umi**, T. Yamada, K. Saito, T. Akiyama*

394. Effective catalyst (cobalt salt/Lewis acid) for Beckmann rearrangement of cycloalkanone oximes. **H. Yamamoto**, A. Ishikawa, M. Sumimoto, K. Hori

Macromolecules, Host-guest Chemistry and Sensors

395. Synthesis of crystal mimicking 1,3-diphenylisobuzofuran. **F. Johansson**, J. Mårtensson*

396. One-pot synthesis of novel polysubstituted 1,1'-phenylene-bipyrrole via the double 1,3-dipolar cycloaddition reaction. **C. Nii**, H. Liu, S. Ueta, F. Yagishita, Y. Kawamura*

397. Development of a new set of quinazolines: Strong fluorophores for solution and solid state. **M. Motoyama**, M. Lukarska, T. Doan, B. Witulski, Y. Suzuki*

398. Synthesis and controlled flapping motion of clothespin-shaped binuclear palladium complexes bearing alkyl amide linkers. **R. Inoue***, S. Kawamori, T. Naota

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401. Biphasic CuAAC reaction using a phase transfer agent. **J. Kim**, S. Lee, Y. Kwon, S. Kim*

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404. Highly efficient synthesis and mono-functionalization of monodisperse poly(ethylene glycols). **Z. Jiang***, H. Zhang, X. Li, Y. Li

405. Synthesis and structure of one-handed M₂L-type helicates made of open-chain hexapyrrole. **T.T. Nguyen**, C. Eerdon, J. Setsune*

406. Membrane fusion triggered by pseudoceramide formation. **S. Lee**, Y. Lee, H. Lee, J. Kim, H. Jeon, S. Kim*

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423. Intra-specific diversity in cytotoxic sesquiterpene lactone constituents of *Eupatorium heterophyllum* collected in P. R. China. **M. Ogata**, Y. Saito, K. Nakashima, Y. Okamoto, M. Tori, T. Kawahara, R. Hanai, Y. Matsuo, T. Tanaka, X. Gong, C. Kuroda

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- 522.** Synthesis of azulenyl amino acids using Petasis reaction. **Y. Tasaki**, T. MURAFUJI*, K. Ishiguro, S. Kamijo
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- 532.** Stereoselective construction of bridged polycyclic systems via a polyene cyclization reaction. **K. Suzuki**, H. Yamakoshi, S. Nakamura*
- 533.** Progress towards the synthesis of lesquerella- and castor-based bisphosphonates. **D.M. Cermak***, S.M. Henry, E.T. Rosen, E.L. Fayer, C.L. Coley, S.C. Cermak*
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- 542.** Enantioselective total synthesis of albaflavonone utilizing sequential intramolecular aldol condensation. **H. Ito***, T. Kobayashi, Y. Kon, H. Abe
- 543.** Formal total synthesis of brevisamide using an oxiranyl anion strategy. **A. Fukuta**, K. Nakamura, M. Nakano, K. Kuroyanagi, T. Sakai, Y. Mori*
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- 545.** Electrochemically promoted divergent synthesis of diterpene. **R. Merchant**, K. Oberg, P.S. Baran

- 546.** Total syntheses of araiosamines A–D. **M. Yan***, M. Tian, J. Shaw, P.S. Baran
- 547.** Efficient total synthesis and biological activity of (-)-bassianolide. **B. Mun**, K. Kim, Y. Lee*
- 548.** Concise total synthesis of broussonone A. **H. Jo**, J. Sim, B. Park, **S. Kim**, H. Lee, J. Jung*
- 549.** Synthetic study of antibacterial natural product citreamicin δ . **R. Sugimura**, E. Takeuchi, Y. Suzuki*
- 550.** Synthetic study of the ABCD fragment of gymnocin-B. **H. Sakakibara**, K. Hata, A. Kawai, R. Ishibashi, T. Sakai, Y. Mori*
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- 558.** Two phase synthesis of the *tigliane* natural products. **H. Chu**, S. Kawamura*, P.S. Baran
- 559.** Chemical conversions of fragmented lignin into lubricant oils. **Q. YE**, Z. Png, M. Chan, X. Wang, C. Wang, P.S. Sudger, J. Xu*
- 560.** Synthesis of glycine phthalimide using a heat gun. **E.A. Brueggeman**, B.W. Baldwin
- 561.** Direct hydroalkylation of unactivated olefins. **H.T. Dao**, C. Li, Q. Michaudel, B. Maxwell, P.S. Baran*
- 562.** Electrochemical functionalization of terpenoid compounds. **B. Rosen***, E.J. Horn*, P.S. Baran

Wednesday Afternoon

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Reactive Intermediates and Unusual Molecules (#7)

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- 13:25 – 564.** Role of nitroxides in the mechanisms of diarylamine radical-trapping antioxidants and hindered amine light stabilizers. **D. Pratt**
- 13:50 – 565.** Reactivation of aged acetylcholinesterase after exposure to organophosphorus chemical nerve agents: A progress report. **C.M. Hadad***
- 14:15 – 566.** Intermediates in the cleavage of endoperoxides. **T. Linker***
- 14:40 – 567.** Mechanism and scope of non-emissive meso-unsaturated BODIPY dyes. **G. Cosa***
- 15:00 – 568.** Series of persistent neutral heavy group-15 element radicals with bulky alkyl substituents. **T. Iwamoto**
- 15:25 – 569.** Synthesis of a stable selenoaldehyde by unprecedented C=C=Se double bond formation through β -dehydration. **K. Goto***, R. Kakimoto, R. Kimura, S. Sase
- 15:50 – 570.** Effect of the substitution of oxygen for CH_2 on the singlet-triplet energy differences (ΔE_{ST}) in trimethylenemethane \rightarrow oxallyl, *meta*-benzoquinodimethane \rightarrow *meta*-benzoquinone and 1,2,4,5-tetramethylenebenzene \rightarrow 1,2,4,5-tetraoxatetramethylenebenzene. X. Wang, B. Chen, D.A. Hrovat, **W.T. Borden***

- 16:15 – 571.** Spectroscopy and kinetics of radical pairs in crystalline ketones. **M.A. Garcia-Garibay***, J. Park, A.J. Ayto
- 16:40 – 572.** Mechanistic study on the stereoselective photodenitration of 2,3-diazabicyclo[2.2.1]heptanes. **M. Abe**

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

Prospects for Flow Chemistry (#29)

Organized by: J. Yoshida, T. Jamison, D. Kim, M. Organ
Presiding: d. kim, M. Oelgemöller

- 13:00 – 573.** Continuous flow synthesis of functional nanomaterials by microreactors and their applications. **d. kim***

- 13:25 – 574.** Continuous flow reactions in synthesis and medicinal chemistry. **A.B. Beeler***, R. Telmesani, T. Lynch-Colameta, A. Courtney-Young

- 13:50 – 575.** Highly efficient organic photo-reactions in flow microreactors under slug-flow conditions. **Y. Nishiyama***, K. Terao, K. Kakiuchi

- 14:05 – 576.** Photochemical transformations using alternative sensitizers in continuous flow. **S. Collins***
- 14:20 – 577.** Enabling scalable photochemical reactions using continuous flow chemistry. **D. Cantillo***, C. Kappe

- 14:35 – 578.** Continuous flow photochemistry: From multistep synthesis to solar chemistry in concentrated sunlight. **M. Oelgemöller**

- 15:00 – 579.** Photochemical transformations accelerated in continuous-flow microreactors. **T. Noel***

- 15:25 – 580.** Development of a novel electrocarboxylation system using a flow microreactor. **H. Tatevo**, K. Nakabayashi, M. Atobe

- 15:40 – 581.** ContiNMR - monitoring and controlling continuous synthesis reactors with benchtop NMR. **S. Riegel**, T. Rehm, J. Barten

- 15:55 – 582.** Vortex fluidic flow chemistry – putting a spin on conventional flow chemistry. **J. Britton**, J.M. Chalker, C. Raston

- 16:10 – 583.** Integrated liquid-liquid separator and its uses in flow chemistry. **a. adamo**

- 16:25 – 584.** Bench-top resistively heated reactor for flow chemistry. **J. Rydfjord**, J. Sävmarkar, M. Larhed*

- 16:40 – 585.** Flow reactors: A paradigm shift. **D. Ager***

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41)

Organized by: T. Akasaka, F. Wudl, L. Echegoyen, X. Lu, C. Wang
Presiding: A. Hirsch, N. Martin

- 13:00 – 586.** Single-molecule and real-time TEM imaging of single organic molecules. **E. Nakamura***

- 13:40 – 587.** Functionalization of synthetic carbon allotropes. **A. Hirsch***

- 14:10 – 588.** New mechanistic insight on top-down vs. bottom-up formation of fullerenes and metallofullerenes. **H.C. Dorn**, J. Zhang, X. Liu, T. Fuhrer

- 14:40 – 589.** $\text{NiO}_{\text{C}60}$: What does the future hold? **K. Pyrakis***

- 15:00 – 590.** Co-assembled-directed fabrication of an exfoliated form of alternating multi-layered composed of self-assembled organoplatinum(II) complex–fullerene dyad. **K. Tashiro***

- 15:20 – 591.** Carbon-rich porphyrins. **N. Jux***

- 15:40 – 592.** Carbonaceous molecular bearings. **H. Isobe**

- 16:00 – 593.** Functionalization of [60]fullerene initiated by palladium-catalyzed C–H activation. **G. Wang***

- 16:20 – 594.** Giant glycofullerenes for biological applications. **N. Martin***

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2

Molecular and Supramolecular Photochemistry (#71)

Organized by: J. Sivaguru, W. Chung, C. Bohne, c. tung, M. Sakamoto, V. Ramamurthy
Presiding: W. Chung

- 13:00 – 595.** Photochemistry of the 1,4-di-phenyl-1,3-butadienes in ethanol – trapping conical intersections. **J. Saltiel***, C.E. Redwood

- 13:30 – 596.** Photochemistry of cyclopropanes: From generation or reactive acetylenes to the development of CORMs. **V. Popik**

- 14:00 – 597.** High contrast reversible solid-state mechano- and thermo-responsive fluorescent materials. **S. Sun***

14:30 Break

- 14:45 – 598.** Turning on the fluorescence of GFP chromophore with meta-amino substituents. **J. Yang***, G. Huang

- 15:15 – 599.** Artificial photosynthetic systems for hydrogen evolution. **L. Wu***

15:45 Break

- 16:00 – 600.** Photochemistry and fluorescence properties of photoresponsive dendrimers and hydrogen bonded compounds. **T. Arai**

- 16:30 – 601.** Take aggregates with a grain of salt. S. Mooi, S. Keller, J. Oake, C. Bohne, B. Heyne*

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74)

Organized by: R. Danheiser, T. Fukuyama, M. Lautens
Presiding: R. Danheiser

- 13:00 – 602.** Gold-catalyzed efficient formation of *N*-heterocycles. **L. Zhang***

- 13:20 – 603.** Selective installation of a sp^3 C–Si bond beta to nitrogen via catalytic silylative reduction of *N*-heteroaromatics. **S. Chang**

- 14:00 – 604.** Cycloadditions of strained alkynes and allenes . **N. Garg***

- 14:40 – 605.** Total synthesis of indoline alkaloids via intramolecular dearomatative oxidative coupling. **D. Ma**, M. Teng, Y. Wei

- 15:20 – 606.** Design and development of bioactive heterocycles: A synergy between synthesis and structural biology. **A.K. Yudin***

- 16:00 – 607.** Efficient synthetic route toward benzofuro[2,3-*b*]pyrroles. **O. Miyata***, M. Ueda, Y. Ito, N. Takeda

- 16:20 – 608.** Direct azidation of phenols with azidoimidazolinium salt. **M. Kitamura***, T. Koga, K. Murakami

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100)

Organized by: D. Hall, B. Wang, P. Duggan, M. Suginome
Presiding: B. Wang

* Principle Author

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13:00 Opening remarks
13:05 – 609. Boronic acid–DMAPO cooperative catalysis for dehydrative condensation of carboxylic acids with amines.
K. Ishihara*, Y. Lu

13:35 – 610. Boronic acid catalysis: An emerging atom-economical platform for direct activation of alcohols in Friedel-Crafts alkylations and other reactions.
D. Hall*, X. Mo, J. Dansereau, J. Yakivchuk, A. McCubbin

13:55 – 611. Synthetic discoveries from polycyclic natural products.
J.A. May*, J. Shih, T. Nguyen, P. Le, R. Vallakati, C. Huynh, t. Tran, S. Jansone-Popova, B. Lundy

14:15 – 612. Copper-catalyzed stereoselective synthesis of organoboron compounds.
J. Yun

14:45 – 613. Synthesis of chiral tertiary boronic esters via oxime-directed catalytic asymmetric hydroboration. V. Shoba, N.C. Thacker, A. Bochat, **J. Takacs***

15:05 Break

15:15 – 614. Anomalous reactivity of silyborane: Boryl substitution of organic halides with silylborane/alkoxy base systems.
H. Ito*

15:45 – 615. Masked boron group as a convertible directing group for transition-metal-catalyzed ortho-C–H functionalization. A. Ishibashi, T. Yamamoto, **M. Sugiyama***

16:05 – 616. Borenium cations: Versatile reagents for the formation of boronate esters.
M.J. Ingleson

16:25 – 617. Small molecule synthesizer.
M. Burke*

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Practical Application of Basic Research on Molecular Recognition (#136)

Organized by: C. Tran, K. Kano, C. Easton
Presiding: C.J. Easton, M. Komiyama

13:00 – 618. Detection and destruction of nerve agents.
J. Rebek

13:25 – 619. QCM sensor arrays as electronic noses for odor recognition.
I.M. Warner, N.C. Speller, N. Siraj

13:50 – 620. Supramolecular tools that enable research on post-translational modifications.
F. Hof*, G. Garnett, A. Shaurya, B. Meagan, K. Daze

14:15 – 621. Supramolecular composite materials: Recyclable synthesis and application.
C.D. Tran*

14:40 Break

14:55 – 622. Direct measurement of interactions involved in biological functions.
K. Kurihara

15:20 – 623. Photochemistry in a capsule: Spin, energy, and electron transfer across a molecular wall.
V. Ramamurthy*

15:45 – 624. Intracellular delivery of the porphyrin-cyclodextrin supramolecular complexes by an octaarginine carrier peptide.
H. Kitagishi*, K. Kano

16:10 – 625. Synthesis and chiral recognition of novel helical poly(phenylacetylene)s having two chiral centers at a pendant.
C. Zhang*, R. Ma, Y. Qiu, Y. Zhou, Y. Okamoto

16:20 – 626. Polyrotaxane synthesizer.
C. Cheng, J. Stoddart*

16:30 – 627. Phospholipid and curvature recognition by designed peptides: A paradigm shift in sensing and capture of extracellular vesicles. B.M. Cook, D.S. Dalisay, **J.P. Saludes***

16:40 – 628. Amphiphilic cyclodextrin thioethers for recognition of hydrophobic drugs.
G. Wenz*, L. Becker

16:50 Closing Remarks

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Molecular Function of Natural Products: Advances towards Chemical Biology (#237)

Organized by: M. Ueda, B. Miller, K. Irie, B. Miller, B. Miller, C. Lin, T. Oishi, C. Forsyth, H. Lee
Presiding: T. Oishi

13:00 – 629. Rational design and discovery of potent siderophore-drug conjugates effective in treating drug-resistant *Acinetobacter baumannii*.
H. Kim*, J. Kim, W. Song, J. Jeong

13:15 – 630. Biochemical analyses of CRBN, the target protein for immunomodulatory drugs (IMiDs).
S. Sakamoto, T. Ito, Y. Yamaguchi, H. Ando, H. Handa*

13:30 – 631. Development of chemical probes for studying mechanism of action of an antitumor saponin OSW-1.
K. Sakurai*, R. Yamada, T. Takeshita, M. Hirazumi

13:45 – 632. Depiction of 3D structure of membrane proteins and assignment of functional subunits using a transmission electron microscopy. M. Mio, M. Tsunoda, **K. Miyo**

14:00 – 633. Total synthesis of cyclodepsipeptide natural products and their biological evaluation.
T. Doi*

14:30 – 634. Natural products possessing stereodefined *N*,*O*-acetals: New synthetic method and molecular function.
Y. Rhee*, S. Wang, w. Lim

15:00 – 635. Marine-derived heterocyclic Ca^{2+} channel agonists: Synthesis, SAR, and chemical biology.
T.F. Molinski*

15:30 – 636. Chemical biology in natural G-quadruplex ligand of telomestatin and its derivatives.
K. Nagasawa*

16:00 – 637. Total synthesis and biological activities of phorbeketals and their analogs.
H. Lee*, S. Joung

16:30 – 638. Total synthesis of natural and non-natural products to probe molecular function.
C. Forsyth*

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Frontiers of Chirality in Organic Chemistry (#286)

Organized by: J. Canary, N. Berova, E. Yashima, M. Hyun, T. Shibata, T. Asahi, C. Welch, S. You
Presiding: T. ASAHI, T. Shibata, C. Welch, S. You

13:00 Introduction

13:05 – 639. Origin of homochirality on prebiotic earth.
R. Breslow*

13:35 – 640. Abundance and distribution of enantiomeric excesses in meteoritic soluble organic compounds.
S. Pizzarello*

14:05 – 641. Asymmetric autocatalysis with amplification of enantiomeric excess and the origin of homochirality.
K. Soai

14:35 – 642. Cooperative catalysis in asymmetric synthesis: Case studies of catalyst design and process innovation.
K. Ding

15:00 Break

15:15 – 643. Chirality mechanisms at the nanoscale.
H. Chen*

15:45 – 644. Nonthermal effect of microwave assisted catalytic enantioselective reactions.
T. Yamada*

16:00 – 645. Novel chiral helical triazole-based C–H – chloride anion-binding catalysts for the enantioselective dearomatization of heteroarenes.
O. Garcia Mancheno

16:15 – 646. Dynamic mirror-symmetry breaking in bicontinuous cubic liquid crystal phases of non-chiral mesogens.
X. Zeng, C. Dressel, M. Prehm, F. Liu, **G. Unger***, C. Tschiertske

16:30 – 647. Vibrational optical activity of cyclic β -helical peptides with opposite chirality: A computational study.
J.R. Cheeseman*, L.A. Nafie

16:45 – 648. Enantioselective synthesis of planar-chiral transition-metal complexes by molybdenum catalyzed asymmetric ring-closing metathesis.
M. Ogasawara*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Fluorinations and Fluoroalkylations (#310)

Organized by: S. Prakash, T. Ritter, K. Mikami, S. Fuster, J. Hu
Presiding: S. Prakash

13:00 Opening Remarks

13:05 – 649. Fluorination and fluoroalkylation of arenes.
J. Hu*, Y. Zeng

13:30 – 650. Selective fluorination strategies.
G. Sandford*

13:55 – 651. Enabling selective fluorinations using designer HF-based reagents.
G.B. Hammond, B. Xu, O.E. Okorombe

14:20 – 652. Sandmeyer-type fluoroalkylations and fluoroalkylthiolations.
L.J. Goossen

14:45 Break

14:55 – 653. Aliphatic C(sp³)-H fluorination.
P. Tang

15:20 – 654. Copper-catalyzed fluorination of arylhalides.
G. Liu*, X. Mu, D. Wang

15:45 – 655. Regio- and enantioselective formation of allylic and benzylic fluorides via transition-metal-catalyzed reactions of trichloroacetimidates and vinyl epoxides with triethylamine trihydrofluoride reagent.
H.M. Nguyen*

16:10 – 656. New advances in F-18 chemistry.
T. Ritter

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Organic Solid-State Chemistry: Structure, Property & Reactivity (#398)

Organized by: M. Sakamoto, L. MacGillivray, J. Vittal
Presiding: R. Bishop, L.R. MacGillivray

13:00 – 657. Generation and amplification of chirality using organic crystals.
M. Sakamoto*, T. Mino

13:30 – 658. Role of sulphur in crystal engineering.
R. Bishop*, M.M. Bhadbhade

14:00 – 659. Explosive co-crystals.
A.J. Matzger

14:30 – 660. Photoresponsive materials for reversibly controlling the properties of surfaces and interfaces.
A. Asadirad, P. Tannour, **N. Branda***

15:00 break

15:10 – 661. Mechanoluminescence of anthracene-based organic salts and co-crystals.
S. Kohmoto*, T. Chuko, Y. Okuda, S. Kosugi, M. Takahashi, H. Masu, K. Kishikawa

15:30 – 662. Monocrystalline polymeric networks.
J. Wuest, D. Beaudoin, O. Levasseur-Grenon, T. Maris

16:00 – 663. Improving the physicochemical properties of solid-state drugs via pharmaceutical co-crystals.
T. Lu

16:30 – 664. Structural studies of hydration/dehydration mechanism of pharmaceutical crystals by ab initio structure determination from powder diffraction data.
H. Uekusa*, K. Fujii, R. Toyoshima

Hilton Hawaiian Village
Tapa Tower, Honolulu Suite 1

Photoredox Catalysis in Organic Synthesis (#440)

Organized by: D. Nicewicz, S. Fukuzumi, W. Xiao

13:00 – 665. Photocatalytic hydroxylation of benzene by the excited state of *p*-benzoquinone derivatives.
K. Ohkubo*, S. Fukuzumi

13:30 – 666. Natural product synthesis using photoredox catalysis.
A. Li

13:50 – 667. Robust platform for photocatalytic organic syntheses using glass-milled microchip.
K. Katayama, S. Kuwahara, K. Yoshida, A. Nakamura

14:10 – 668. New avenues in synthesis via organic photoredox catalysis.
D. Nicewicz

14:40 Break

14:50 – 669. High-throughput photocatalysis in the development of green manufacturing processes.
D. DiRocco

15:20 – 670. Synthesis of aza-arenes using visible light-promoted radical isocyanide insertions.
S. Yu*

15:50 – 671. Visible light-driven photoredox catalysis in the construction of heterocyclic ring systems.
W. Xiao

16:20 – 672. Discovery and invention of new chemical reactions using photoredox catalysis.
D. MacMillan

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

Catalytic Multicomponent, Tandem and Cascade Reactions (#455)

Organized by: B. Arndtsen, J. Montgomery, K. Nozaki
Presiding: B. Arndtsen, J. Montgomery, K. Nozaki

13:00 – 673. Arylation of weakly acidic C–H's with heterobimetallic catalysts.
P.J. Walsh*

13:30 – 674. Copper-catalyzed oxidative de-carboxylation of phenyl acetic acids under O₂ atmosphere.
Q. Song

13:50 – 675. Tandem reactions mediated by visible light photoredox catalysis.
C. Stephenson*

14:20 – 676. Synthesis of 3-diazoindolin-2-imines through cascade copper catalysis and their utility as cyclized α -imino rhodium carbene precursors.
P. Lyu*, Y. Wang

14:40 – 677. Multicomponent multicatalyst reactions:
(MC)2R. **M. Lautens**

15:10 Break

15:20 – 678. Rhodium-catalyzed chemo-, regio-, and enantioselective cross-trimerization reactions of three different unsaturated compounds.
K. Tanaka

15:50 – 679. Sequentially Pd- and Pd-Cu-catalyzed one-pot syntheses of heterocycles.
T.J. Müller*

16:10 – 680. Diversity-oriented synthesis of chiral heterocycles via enantioselective multicomponent reactions and postcyclizations.
M. Tang, L. Qiu, S. Liu, W. Hu*

16:30 – 681. Merging palladium catalyzed tandem and multicomponent coupling reactions.
B. Arndtsen*

Wednesday Evening

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Reactive Intermediates and Unusual Molecules (#7)

Organized by: R. Sheridan, M. Abe, W. Leigh

19:00 – 682. Structure and reactivity of cyclophanes derived from reactive bis(isobenzofuran)s.
P.W. Dibble*, R. Wells, C. Kurtz, C. Willoughby, K. Fischer, R. Boeré

19:20 – 683. Properties of unusual anionic amides, amides bearing two heteroatoms at nitrogen.
S.A. Glover*, A. Rosser

19:40 – 684. Asymmetric open-shell molecular systems: Remarkable nonlinear optical responses and their spin state dependences.
M. NAKANO*, K. Fukuda, S. Ito, Y. Minamida

* Principle Author

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- 20:00 – 685.** Selectivities in nucleophilic additions to a *p*-benzyne and in the quenching of the resulting aryl anion.
C.L. Perrin*, G.J. Reyes-Rodriguez
- 20:20 – 686.** Novel annelated semibullvalenes: Strain dynamics and homoaromaticity.
R.V. Williams*, A.J. Aring, M.C. Bonifacio

Hawaii Convention Center
Halls I, II, III

Prospects for Flow Chemistry (#29)

Organized by: J. Yoshida, T. Jamison, D. Kim, M. Organ

Poster Session 19:00 – 21:00

- 687.** Porous polymer monolith applied to reactor for organic synthesis. **N. Ishizuka***, K. Mitamura, S. Watase, K. Matsukawa
- 688.** Polyfunctional carotenoid synthesis via one-pot strategy: Toward elucidation of highly efficient energy transfer by marine photosynthetic organisms.
K. Sakaguchi*, T. Kajikawa, S. Hananuki, N. Kinashi, D. Kosumi, H. Hashimoto, H. Frank, T. Shinoda, S. Katsumura*
- 689.** Dehydration of alcohols in a flow system using acid-functionalized silica gel: Application to the synthesis of pristane. **Y. Hirobe**, A. Furuta, T. Fukuyama, I. Ryu*, Y. Manabe, F. Koichi
- 690.** Metal-catalyzed amination processes in continuous flow synthesis. **H. Piras**, H. Lebel*
- 691.** Highly efficient asymmetric photoreactions by flow microreactors.
Y. Nishiyama*, K. Terao, K. Kakiuchi
- 692.** Applying flow chemistry for hydrogenation of four N_4 -tetradentate ligands.
A. Bjelosevic, M.R. Kriss, C. Gordon, J. Aldrich-Wright*
- 693.** Integration of aerobic oxidation of alcohols and unsaturated bond formation catalyzed by polymer-incarcerated metal nanoparticle catalysts. **A. Suzuki**, H. Miyamura, T. Yasukawa, S. Kobayashi*
- 694.** Flash generation and borylation of trifluoromethylvinyllithium and its application to cross-coupling. **T. Fujita**, N. Konno, Y. Watabe, T. Ichitsuka, A. Nagaki, J. Yoshida, J. Ichikawa*
- 695.** Flow chemistry: Developments and applications. **G. Tramper***
- 696.** One-shot double amination of Sondeheimer-Wong dynes. **A. Orta***, F. Xu, K. Shinohara, T. Nishida, S. Ohta, K. Tomiyama, J. Otera
- 697.** Dirhodium(II) complex-catalyzed enantioselective carbonyl ylide cycloaddition reactions under continuous flow conditions. **K. Takeda**, A. Hirota, M. Anada, S. Hashimoto*
- 698.** Kinetically controlled Fischer glycosylation using acidic silica-gel under fluidic conditions. **S. Masui**, Y. Manabe, A. Shimoyama, T. Fukuyama, I. Ryu*, K. Fukase*
- 699.** Soft ruthenium and hard Bronsted acid combined catalyst for efficient cleavage of allyloxy bonds toward protecting chemistry. **S. Tanaka**, Y. Suzuki, H. Saburi, M. Kitamura*

Hawaii Convention Center
Halls I, II, III

Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41)

Organized by: T. Akasaka, F. Wudl, L. Echegoyen, X. Lu, C. Wang
Presiding: X. Lu, C. Wang

Poster Session 19:00 – 21:00

- 700.** Novel metal–carbon hybrid molecules: Endohedral metallofullerenes. **X. Lu***
- 701.** Light scattering characterizations of mesoscale aggregation properties of C_{60} in aromatic solvents. **R. Guo***, C. Hu*, S. Chen
- 702.** Carbon nanotubes: Biopolymers composite materials. **A. Aldalbahi***

- 703.** Regioselective syntheses and crystal structures of fullerene-pentacene mono-adducts. **H. Shirai**, T. Tajima, T. Inui, T. Nishihama, Y. Takaguchi*
- 704.** Designing and guiding the synthesis of inherently nanostructured carbon-based thin films. **G. Gueorguiev**
- 705.** Synthesis of novel pyridine/pyridinium-type fullerene derivatives with human immunodeficiency virus-reverse transcriptase inhibition activity. **T. Yasuno**, K. Takahashi, T. Ohe, S. Nakamura, T. Mashino*
- 706.** Synthesis of multitarget fullerene derivatives with both HCV RNA polymerase inhibitory and antioxidant activities for the treatment of HCV-related disease. **H. Kataoka**, K. Takahashi, T. Ohe, S. Nakamura, T. Mashino*
- 707.** [2+2] Cycloaddition of coumarin derivatives with fullerene under photo-irradiated conditions. **M. Hayama**, M. Ueda, S. Yoshida, H. Yasuda, I. Ryu*
- 708.** Far-UV absorption spectroscopy of linear polyyne molecules in solutions. **Y. Wada***, Y. Morisawa, T. Wakabayashi, Y. Ozaki
- 709.** Hydrogen evolution using a supramolecular photosensitizing system based on the (6,5)single-walled carbon nanotubes. **Y. Tango**, Y. Takaguchi*, K. Kurniawan, T. Tajima
- 710.** [2+2] Cycloaddition of aromatic allenes with C_{60} . **M. Ueda***, S. Yoshida, H. Yasuda, I. Ryu
- 711.** New functionalization approaches for trimetallic nitride metallofullerenes. **T. Li**, L. Bai, H.C. Dorn*
- 712.** Ortho and para water encapsulated in C_{60} : Infrared spectroscopy study. **T. Room***, A. Shugai, U. Nagel, S. Mamone, M.H. Levitt, A. Krachmalnicoff, R.J. Whitley, Y. Murata, J. Li, N.J. Turro
- 713.** Synthesis, properties, and structure of functionalized cycloparaphenylenes. **Y. Miyachi**, K. Tanaka*
- 714.** Regioselectivity of sp^3 defects and brightening of carbon nanotube photoluminescence: Theoretical perspective. **G. Juhasz***, N. Nakashima
- 715.** Enantiospecific formation of fulleropyrrolidines. **M. Garcia Borràs***, S. Osuna, K.N. Houk, M. Solà
- 716.** Surface modification of HOPG and graphene by rod-shaped mixed-valence Ru complexes. **N. Katori**, T. Kita, H. Ozawa, M. Haga
- 717.** Chemical reduction of metallofullerene $La@C_{60}$ by electron donors. **Y. Sato***, K. Akiyama, S. Kubuki
- 718.** Regioselective synthesis of novel multifunctionalized fullerenes by a substitution reaction of halogenofullerenes. **K. Watanabe**, K. Uchiyama, H. Takahashi, K. Yoza, H. Moriyama*
- 719.** Coronene-based supramolecular rotors. **Y. Yoshida***, Y. Kumagai, M. Mizuno, K. Isomura, H. Kishida, G. Saito
- 720.** Synthesis and evaluation of new type of water-soluble fullerene materials. **T. Endo***, Y. Yamaoka, E. Kwon
- 721.** Noncovalent functionalization of multi-walled carbon nanotubes with hydroxyl group containing pyrene derivatives: Molecular structure effects of pyrene derivatives on the properties of polycarbonate composites. **E. Choi***, J. Kim, Y. Jo, c. Kim
- 722.** Regioselective Diels-Alder reaction of ketolactam open-cage fullerenes. **T. TANAKA***
- 723.** Multidimensional NMR studies of fullerene bisadduct regiosomers. **Y. Wan**, G. Liu, T. Yang, N. Chen*, X. Li*
- 724.** Synthesis and NMR properties of H_2 - and H_2O -encapsulating aza[60]fullerenes. **Y. Hashikawa**, M. Murata, A. Wakamiya, Y. Murata*
- 725.** Properties and dynamics in fullerol-based-composites studied by solid-state NMR. **Y. Sano**, H. Ogata
- 726.** Radical spin interaction of graphene flake embedded into h-BN sheet. **M. Maruyama***, S. Okada
- 727.** Structural dependence of electronic properties of graphene nanoribbons on an electric field. **A. Yamamoto***, S. Okada
- 728.** Geometric and energetics structures of corannulene polymers. **K. Narita**, S. Okada
- 729.** Gate voltage variation for carrier accumulation by the defects in carbon nanotubes. **U. Ishiyama***, S. Okada
- 730.** Viologen embedded polyaromatic hydrocarbons: Synthesis and characterization. **E.L. Clelland***, X. Zhang, T. Bakupog
- 731.** Structural properties of 1D fullerene polymer studied by Raman spectroscopy and density functional theory calculation. **A. Takashima***, T. Nishii, J. Onoe
- 732.** Host-guest complexation and TEM imaging of cyclodextrins on nanocarbon surface. **J. Yamada***, A. Kumamoto, N. Shibata, K. Harano, E. Nakamura
- 733.** Theoretical investigation of small molecule adsorption on graphitic surfaces. **C. Squire**, J.D. Head
- Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 2
- Molecular and Supramolecular Photochemistry (#71)**
- Organized by: J. Sivaguru, W. Chung, C. Bohne, c. Tung, M. Sakamoto, V. Ramamurthy
Presiding: M. Sakamoto
- 19:00 – 734.** Photochemical and photophysical processes in aqueous dendritic media. **N. Jayaraman***, B. Natarajan, S. Gupta, B.M. Kiran, J. Nithyanandhan, V. Ramamurthy*
- 19:30 – 735.** Singlet oxygen and antioxidant model substrates. **A.G. Griesbeck***
- 20:00 – 736.** Studying mechanism in photo-redox catalysis. **T.P. Yoon***
- 20:30 – 737.** Structure effect of organic dyes for sensitized solar cells. **T.J. Chow***
- Hawaii Convention Center
Halls I, II, III
- Innovative Strategies for the Synthesis of Nitrogen Heterocycles (#74)**
- Organized by: R. Danheiser, T. Fukuyama, M. Lautens
Presiding: M. Lautens
- Poster Session**
19:00 – 21:00
- 738.** Asymmetric synthesis of crambescin B carboxylic acid, a potent inhibitor of voltage-gated sodium channels, and its analogs. **Y. Nakane**, Y. Ishikawa, A. Nakazaki, T. Nishikawa
- 739.** Synthetic studies of carbazole alkaloids. **H. Yokoyama***, M. Miyazawa
- 740.** Oxidative cyclization of 1-(pyridin-2-yl)-guanidine derivatives: A synthesis of [1,2,4]triazolo[1,5-*a*]pyridin-2-amines and an unexpected synthesis of [1,2,4]triazolo[4,3-*a*]pyridin-3-amines. **K. Ishimoto***, T. Nagata, M. Murabayashi, T. Ikemoto
- 741.** Transition metal-free amination using bench stable N-linchpin reagents. **P.V. Kattamuri**, L. Kurti*
- 742.** Transition metal-free direct primary amination of aryl halides with renewable aminating reagents. **H. Gao**, L. Kurti*
- 743.** Synthetic studies towards the total synthesis of daphlongeranine B. **Y. Ogura***, D.J. Dixon*
- 744.** Inverse regioselective 1,3-dipolar cycloaddition by means of carbonyl *umpolung*. **Y. Hashimoto**, H. Ishiwata, M. Katoh, S. Tachikawa, M. Sekino, S. Ban, N. Morita, O. Tamura*
- 745.** Library construction for thiazole fused-diazepine derivatives using traceless solid-phase synthesis. **D. Lee**, D. Baek, T. Kim, J. Kim, W. Lee, S. Kwak, J. Bae, T. Lee
- 746.** Solid-phase synthesis 2,4-disubstituted 5-carbamoyl-thiazole derivatives. **J. Kim**, D. Kim, D. Lee, S. Kim, Y. Gong*, T. Lee*
- 747.** Solid-phase synthesis of multi-substituted xanthine derivatives. **T. Kim**, S. Lee, D. Lee, S. Kim, S. Lee*, T. Lee*
- 748.** Synthesis of 2-aminobenzoselenazoles from bis(2-aminodiphenyl) diselenides and isothiocyanates. **H. Ichikawa***, N. Miyashi, S. Shimizu
- 749.** Copper-catalyzed one-pot synthesis of indoles from anilines and propargyl acetates. **K. Enomoto**, M. Takayanagi, T. Konakahara, Y. Ogiwara, N. Sakai
- 750.** Exploiting weak N–N bonds: New synthetic approaches to functionalized biaryls and an acid-free Fischer indole synthesis. **C. Keene**, L. Kurti*
- 751.** Novel rare earth metal-catalyzed synthesis of benzaozoles. **S. Naito**, T. Yoshimura, Y. Kimura, A. Toshimitsu, T. Kondo*
- 752.** Efficient solution-phase synthesis of 1,3,4-oxadiazoles and 1,3,4-thiadiazole derivatives through reagent-based cyclization process of thiocsemicarbazide intermediate. **s. yang***, H. Yoo*, Y. Gong*
- 753.** Suzuki-Miyaura reactions of 2,6-diethoxyprydines with alkyl boronic esters. **J.L. Roizen**
- 754.** Reductive synthesis of indolinone derivatives using carbon dioxide. **I. Kurata**, T. Amaya, T. Hirao
- 755.** Synthesis of 4(3*H*)-quinazolinones by $Yb(OtF)_3$ -catalyzed heterocyclization reactions of 2-aminobenzamides with 1,3-dicarbonyl compounds. **T. Yoshimura***, Y. Kimura, A. Toshimitsu, T. Kondo
- 756.** Iron-catalyzed enantioselective carbonmetalation of azabicyclic alkenes with arylzinc reagents. **S. Saito***, K. Isozaki, L. Adak, N.J. Gower, P. Cogswell, T. Kawabata, M. Jin, T. Itoh, S. Ito, M. Nakamura
- 757.** Reaction of 2-pentene-1,4-dione with heterocyclic compounds in the presence of $BF_3\cdot OEt_2$ and the related reaction. **S. Kawabata***, H. Nishino
- 758.** Total synthesis of grandioline C and related *Kopsia* alkaloids. **M. Nakajima**, S. Arai, A. Nishida*
- 759.** Synthesis of functionalized 2-oxindoles by Friedel-Crafts reactions. **M. Gasono**, D.A. Klumpp*
- 760.** Cascade reactions of amido-acetals in superacid: A synthetic route to indolizidines and quinolinizidines. **A. Qarah**, A. Tracy, A. Kethe, D.A. Klumpp*
- 761.** Palladium-catalyzed oxidative cyclization of alkenes/alkynes to construct nitrogen heterocycles. **J. Zheng**, W. Wu*, H. Jiang*
- 762.** Modified synthesis of quinine and quinidine. **Y. Kobayashi***, Y. Kaneko, N. OGAWA
- 763.** Diversity-oriented syntheses of indoline-based novel heterocycles. **Y. Jung**, I. Kim*
- 764.** Synthesis of isoxazoles from conjugated silyl nitronates. **A.J. Doue**, I.R. Pottie*
- 765.** Synthesis of 1*H*-1,2,3-triazolecarboxylates. **C. Butler**, r. henry, A.M. Schöffstall
- 766.** Selective synthesis of 2,3-disubstituted indoles via a dimetallic intermediate. **M. Isomura**, L. Ilies, M. Nakamura, E. Nakamura*
- 767.** Copper-catalyzed [4+2] cycloaddition of *N*-(2-pyridyl)ketimines and alkynes. **K. Tatsumi**, T. Fujihara, J. Terao, Y. Tsuji*

* Principle Author

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- 768.** Fluorinated and trifluoromethylated disubstituted 1*H*-1,2,3-triazoles.
A.M. Schoffstall, D.A. Clarke,
L.F. George, W.A. Robertson,
K.A. Knobbe
- 769.** Direct and catalytic guanidination of amino groups by $\text{Sc}(\text{OTf})_3$ in water.
K. Tsubokura*, T. Iwata*, Y. Nakao,
K. Tanaka*
- 770.** Synthesis of multisubstituted pyrroles via copper-catalyzed condensation of imines and diazocarbonyl compounds.
S.W. Tan, N. Yoshikai
- 771.** Rapid synthesis of tri/tetraaryl-substituted pyrazoles via [3+2] cycloaddition and C–H direct arylation approaches.
T. Morita, S. Fuse*, K. Matsumura,
H. Sugiyama, D. Kobayashi, H. Tanaka,
H. Nakamura, T. Takahashi
- 772.** Total syntheses of 1988 B and C.
S. Sato, A. Hirayama, H. Ueda,
H. Tokuyama*
- 773.** Indium-catalyzed reductive annulation of keto acids with primary amines leading to *N*-substituted lactams. **T. Uchiyama**,
Y. Ogiwara, N. Sakai
- 774.** One-pot approach to 2-arylbenzoxazinone derivatives using copper-mediated oxidative tandem reactions.
M. Yamashita*, Y. Nishizono, A. Iida
- 775.** Novel 3-substituted-1,10-phenanthroline via high yielding microwave assisted Friedländer condensation using aldehydes. **G.H. Dennison***, M.R. Johnston*
- 776.** Experimental and computational mechanistic evaluation of a palladium-catalyzed ring expansion of spirocyclic δ -lactams and piperidines. **O. René***,
I.A. Stepek, A. Gobbi, B.P. Fauber,
S. Gaines
- 777.** Asymmetric synthesis of quinolizidine, indolizidine, and pyrrolizidine azabicycles. **I. Houbly***, S. Davies,
A. Fletcher, E. Foster, P. Roberts,
T. Schofield, J. Thomson
- 778.** Nitrosallenenes: New reactive species for umpolung functionalization and heterocycles synthesis. **H. Tanimoto***,
K. Yokoyama, T. Shitaka, Y. Mizutani,
K. Kakuchi
- 779.** Asymmetric synthesis of chiral diamines by formal imino cyclization.
A.R. Pradipta, K. Tanaka*
- 780.** Chiral holmium complex-catalyzed asymmetric Diels-Alder reaction of silyoxybutadienes and enantioselective total synthesis of (–)-minovincine.
T. Morikawa, S. Harada, A. Nishida*
- 781.** Stereodivergent synthesis of chiral β -lactams through the enantioselective reduction of iminocyclobutenones and the subsequent thermal rearrangement of aminocyclobutenones. **I. Hachiya***,
M. Shimizu
- 782.** Dehydrosulfurative C–N cross-coupling and concomitant oxidative dehydrogenation of 3,4-dihydropyrimidin-1*H*-2-thiones for general synthesis of 2-aminoypyrimidine derivatives. **J. Sohn***, N. Phan
- 783.** Towards dephospho form A. **A. Klewe**,
T. Lindel*
- 784.** Conversion of alcohols into value-added nitrogen containing heterocycles via ruthenium-catalyzed hydrogen transfer coupling strategy. **M. Zhang**
- 785.** Rapid access to 3-aminoindazoles from tertiary amides. **W.S. Bechare***,
S. Régnier, P. Cyr, A.B. Charette
- 786.** Progress towards the total synthesis of callosine. **M. Vriesen***, M.A. Kerr
- 787.** Negishi approach to 1,5-disubstituted 3-amino-1*H*-1,2,4-triazoles. **H. Zhang**
- 788.** Base- and additive-free approach of the Tsuji-Trost reaction for the synthesis of nitrogen heterocycles. **M. Kljajic**,
R. Breinbauer
- 789.** Rh-catalysed carbonylation of non-activated aziridines to β -lactams at low CO pressure mediated by an unusual electron rich phosphine ligand. **C. Buxton***,
D. Blakemore, J. Bower
- 790.** U.V. light mediated synthesis of carbazoles using flow chemistry. **A. Caron**,
A. Hernandez-Perez, S. Collins*
- 791.** Enantioselective, catalytic anhydride-Mannich reaction: Efforts toward the synthesis of 7-deoxypancratistatin.
M.J. Di Maso, S. Laws, J.T. Shaw

- 792.** Synthesis of polyring-fused amines via stereoselective seleno-Claisen rearrangement. **F. Shibahara***, M. Suzuki,
S. Kubota, T. Murai
- 793.** Development and application of Pd-catalyzed cross-coupling methods for the parallel synthesis of nitrogen heterocycles. **A. Capretta***
- 794.** Ring-opening cyclization of spirocyclopropanes with amines: rapid access to 2-substituted 4-hydroxyindoles.
H. Nambu, M. Fukumoto, W. Hirota,
T. Yukura
- 795.** Studies toward the synthesis of pyrroloindole natural products.
J.E. Curiel Tejeda, M.A. Kerr*
- 796.** Enantioselective synthesis and functionalization of nitrogen heterocycles through olefin hydroacylation reactions.
L.M. Stanley
- 797.** Highly efficient one-pot double cyclizations in the asymmetric syntheses of polyfunctionalized azabicycles.
M. Brambilla*, S. Davies, A. Fletcher,
P. Roberts, J. Thomson
- 798.** Enantioselective dearomatic [3+2] cycloadditions of azometathine ylides and electron-deficient arenes and heteroarenes. **A. Gerten**, L.M. Stanley*
- 799.** Synthesis of tricyclic benzazonines byaza-Prins reaction. **T. Katamura***,
T. Shimizu, Y. Mutoh, S. Saito
- 800.** Development of a hypervalent iodine mediated ring contraction of lactams and its application towards the synthesis of alkaloids. **S. Aubert-Nicol**, C. Spino*,
J. Lessard
- Hawaii Convention Center
Halls I, II, III
- Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100)**
- Organized by:* D. Hall, B. Wang,
P. Dugan, M. Sugiyama
Presiding: D. Hall
- Poster Session**
19:00 – 21:00
- 801.** Conversion of potassium organotrifluoroborates to organoborohydrides.
E.R. Abbey*, C. Bateman, H. Beal,
J. Arakawa, D. Donovan
- 802.** Unprecedented catalytic use of gallium(0) in organic synthesis. **B. Qin**,
U. Schneider
- 803.** "Super activated" lithium cation based on carborane anions and its novel reactivity. **V. Kitazawa***, R. Takita,
S. Matsubara, M. Uchiyama
- 804.** Byproduct free synthesis: Radical cyclization of NHC-boranes and decyanation of malononitriles. **T. Kawamoto**,
D.P. Curran*
- 805.** Hydrazone-palladium catalyzed one-molecular alkylic arylation. **K. Watanabe**,
T. Mino*, M. Sakamoto
- 806.** Copper salt catalyzed addition of arylboronates to azodicarboxylate.
T. Uemura, **M. Yamaguchi**, N. Chatani*
- 807.** Complementary synthesis of borylated N-heterocycles. **C. Merlic***,
R. Tobolowsky
- 808.** Ruthenium-Me-BIPM catalyzed asymmetric addition of arylboronic acids to synthesis of chiral benzofuranone derivatives. **M. Yohda**, Y. Yamamoto*
- 809.** Cyclic ketones synthesis by intramolecular acylation of organocobalt with esters. **T. Ueno**, Y. Suyama, M. Ueda*, I. Ryu*
- 810.** Facile $\text{Me}_3\text{SiNR}'$ -catalyzed enolate isomerization enables a general method for stereoselective synthesis of enol boronates by borylation of lithium enolates. **D. Kundu**, D. Ward*
- 811.** Synthesis of 1,4-enynes by catalyst-free coupling reaction of alkynylboronic acids with secondary propargylic acetates. **D. Nakakoji**
- 812.** Base catalysed bora-Brook rearrangement: The effects of solvent polarity, the backbone of boryl group, and counter cation of base toward reaction rate.
H. Kisu, M. Yamashita*, K. Nozaki*,
H. Sakaino, F. Ito
- 813.** Azaborines: Novel core isosteres for heteroaromatic systems. **G.H. Davies**,
G.A. Molander
- 814.** Regioselective diboration using unsymmetrical diborane(4) in the absence of transition metal catalyst. **C. Kojima**,
M. Yamashita*
- 815.** Diastereoselective allylation of imines and hydrazones using allylboronic acids: Scope and mechanistic investigation.
R. Alam*, A. Das, K.J. Szabo
- 816.** Two-photon induced photobleaching in conjugated organoboron compounds.
H. Haruno, Y. Kurakami, M. Kato,
S. Fukushima, H. Ito, M. Fujino*
- 817.** Copper-catalyzed C–N bond formation between boronic acids and organic azides at room temperature. **W. Kim***
- 818.** Nickel-catalyzed borylation of aryl 2-pyridyl ethers through the cleavage of a carbon–oxygen bond. **M. Tobisu***,
J. Zhao, H. Kinuta, N. Chatani
- 819.** Rhodium-catalyzed cross-coupling of aryl carbamates with organoboron reagents. **K. Yasui**
- 820.** Nickel-catalyzed transformation involving the cleavage of a carbon–nitrogen bond in aniline derivatives. **M. Tobisu***,
K. Nakamura, N. Chatani
- 821.** Catalytic arene borylation based on *in situ*-generated boreniun species.
F. Kitani*, T. Imahori, R. Takita,
M. Uchiyama
- Hawaii Convention Center
Halls I, II, III
- Practical Application of Basic Research on Molecular Recognition (#136)**
- Organized by:* C. Tran, K. Kano,
C. Easton
- Poster Session**
19:00 – 21:00
- 822.** Formose reaction in the presence of water soluble polymers. **T. MICHTAKA***,
A. Hashidzume, T. Sato
- 823.** Highly active bifunctional triporphyrin catalysts for CO_2 fixation. **K. Ogawa**,
C. Maeda, T. Taniguchi, T. Ema
- 824.** Chiral recognition of sympathetic β -blocking agent propranolol using (-)-epigallocatechin-3-O-gallate.
H. Tsutsumi, E. Yokoyama, T. Ishizu*
- 825.** Control of formose reaction using phenylboronic acid residue. **T. Imai**,
A. Hashidzume, T. Sato*
- 826.** Tunable solid-state fluorescent materials for supramolecular encryption.
X. Hou, C. Ke, J.F. Stoddart*
- 827.** Molecular tetrahedron. **J. Sun**, Y. Wu,
J.F. Stoddart*
- 828.** Synthesis of cyclophane oligomers by RAFT polymerization and their host-guest properties. **K. Nakamura**
- 829.** Selective DNA-binding small-molecule fluorescent probes for live cell imaging.
V. Thangavel, G. NAMASIVAYAM,
T. Bando, H. Sugiyama
- 830.** Developing surface imprinted polymers for selective recognition of pharmaceutical targets. **A. Mujahid***, S. Roshan,
S. Bajwa, A. Afzal, N. Iqbal, T. Hussain
- 831.** Synthesis and evaluation of naphthyridine derivatives having amino sugar.
H. Aikawa, Y. OKADA, H. Ito,
K. NAKATANI*
- 832.** New Cu^{2+} -selective fluorescent probe based upon dansyl derivative and its applications. **M. Choi**, J. Hong, I. CHANG,
S. Chang*
- 833.** Shape-persistent cavities of a rigid dendrimer. **Y. Kato**, T. Kambe, T. Imaoka,
K. Yamamoto*
- 834.** Syntheses and developments of polydiacetylene-based chemosensors. **S. Lee**,
J. Yoon*
- 835.** Structural optimization of bifunctional metallocorphyrin catalysts for CO_2 fixation. **C. Maeda**, J. Shimonishi, K. Ogawa,
T. Ema
- 836.** Cyanine based near-infrared fluorescent sensor and its bioimaging application. **Y. Hu**, J. Yoon*
- 837.** Biological imaging of mitochondria in various way by using a cyanine derivative probe. **Y. BAEK**, k. kim, J. Yoon*
- Hawaii Convention Center
Halls I, II, III
- Homogeneous Gold Catalysis: Methods, Theories and Applications (#192)**
- Organized by:* L. Zhang, H. Ohno, R. Liu
Presiding: L. Zhang
- Poster Session**
19:00 – 21:00
- Natural product synthesis**
- 838.** Gold(I)-catalyzed cascade cyclization of enediynes to 6*H*-dibenzo[c,h]chromen-6-ones. **M. Wu***
- 839.** Gold alkene pi-complexes: Ligand effects on structure, formation and reactivity. **A.C. Jones**, C. Griebel, J. Piedad,
W. Zhou
- 840.** Gold-catalyzed sequential [3+2]/[3+2] cycloadditions cascade of *N*-alkoxyazomethine ylide. **M. Ueda***,
S. Sugita, N. Takeda, O. Miyata*
- 841.** Total syntheses of hyperforin, papauarin A-C and formal synthesis of nemorosone: Toward the the total synthesis of ginkgolides. **G. Bellavance**,
L. Barriault*
- 842.** Catalytic reaction with AuNPs/ π -conjugated diblock copolymers (II) – oxidation reactions of benzhydrol. **H. Furukawa**,
M. Fujita, Y. Takeoka, M. Rikukawa
- 843.** Silver-Ccatalyzed C–C bond formation with carbon dioxide. **T. Yamada**
- 844.** Synthesis and reactivities of pyridyl-gold complexes bearing alkyne moiety. **H. TAKEMOTO**, N. NISHINA*
- 845.** Three-component domino process for the pyrrolizine skeleton via [3+2]-cycladdition of azomethine ylide and enamino cyclization triggered by a gold catalyst. **K. Sugimoto**, N. Yamamoto,
D. Tominaga, Y. Matsuya*
- 846.** Gold-catalyzed cyclization-rearrangement reaction for the synthesis of 3-hydroxyisoxazoles. **S. Sugita**, M. Ueda*,
K. Noguchi, N. Takeda, O. Miyata*
- 847.** Regioselective cis insertion of DMAd into Au–P bonds: Effect of auxiliary ligands on reaction mechanism.
T. NAKAJIMA, H. Kuniyusa, T. TAMAKI,
T. Iwasaki, N. Kambe
- 848.** Synthesis of angular and fused polycyclic compounds with Au(I) catalyst. **P. McGee**, L. Barriault*
- 849.** Light initiated cascade reaction for the synthesis of polycyclic compounds.
M.A. Morin, L. Barriault*
- 850.** Au(I)-catalyzed cyclization: Its application to the syntheses of polyethers.
M. Matsuo, M. Miyazawa, H. Yokoyama*
- 851.** Gold-catalyzed cycloisomerization of medium-sized cyclic ethers. **M. Kubota***,
T. Saito, M. Uchiyama
- 852.** Pd-catalyzed asymmetric intermolecular addition of homopropargylic alcohol to alkoxycallene: Development and application. **J. Kim**, W. Lee, Y. Rhee*
- 853.** Synthesis and structure of phosphine-gold complexes bearing alkynyl moiety. **F. KIMURA**, N. NISHINA*
- 854.** Liquid phase benzene hydroxylation over copper binuclear complex catalysts. **K. Kata**, A. OKEMOTO, K. Taniya,
Y. ICHIHASHI, S. NISHIYAMA
- 855.** Gold-catalyzed cascade reaction of 1,7-dienes: Applications in collective synthesis of cladiellins. **G. Yue**, **J. Gong**,
T. Luo*, Z. Yang*

* Principle Author

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856. Gold catalyzed allene's cycloaddition and cyclization reaction. **Z. Chen**

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Molecular Function of Natural Products: Advances towards Chemical Biology (#237)

Organized by: M. Ueda, B. Miller, K. Irie, B. Miller, B. Miller, C. Lin, T. Oishi, C. Forsyth, H. Lee

19:00 – 857. New prespore-cell-promoting factor of cellular slime molds, *Dictyostelium discoideum*. **Y. Takaya***, R. Hotta, K. Fujiwara, M. Niwa, K. Inouye, A. Oohata

19:12 – 858. Isolation and evaluation of an ability to bind to protein kinase C of (20S)-bryostatin 19 from Japanese bryozoan: Elucidation of the role of the side-chain at C-20. **R.C. Yanagita**, K. Muraki, M. Takata, Y. Kawanami, K. Irie

19:24 – 859. Hepatitis C virus cell culture system identifies fungi-derived NeoB (SF30) as a liver X receptor inhibitor. **K. Watahi***

19:36 – 860. Sterol degradation pathway in *Mycobacterium tuberculosis* is a target of secondary metabolites from Philippine plants. **A.P. Tolones**, S. FRANZBLAU, M.J. Garson, A. Aguinaldo*, J.P. Saludes*

19:48 – 861. Total synthesis and 3D structural analysis of aprotocixin C. **Y. Masuda**, J. Suzuki, Y. Onda, M. Yoshida, T. Doi*

20:00 – 862. Synthesis and biological evaluation of hibiscosic C. **B.C. Goess***

20:12 – 863. Structure–activity studies on the PKC-recognition domain of aplysin toxin, a potent tumor-promoter isolated from a sea hare. **Y. Ashida**, R.C. Yanagita, C. Takahashi, M. Fujii, Y. Kawanami, K. Irie

20:24 – 864. 5-Alkyl-1,2,3,4-tetrahydroquinolines (5aTHQs), new membrane-interacting lipophilic metabolites, produced by combined-culture of *Streptomyces nigriceps* and *Tsukamurella pulmonis*. **R. Sugiyama***, S. Nishimura, T. Ozaki, S. Asamizu, H. Onaka, H. Kakeya

20:36 – 865. Total synthesis and structure-activity relationship of ormaezallene toward the development of molecular probe for antifouling substance. **T. Umezawa***, E. Yoshimura, Y. Nogata, T. Okino, F. Matsuda

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Frontiers of Chirality in Organic Chemistry (#286)

Organized by: J. Canary, N. Berova, E. Yashima, M. Hyun, T. Shibata, T. Asahi, C. Welch, S. You
Presiding: J. Canary, C. Welch

19:00 – 866. Practical catalytic hydrogenation. **X. Zhang***

19:15 – 867. Enantioselective and diastereoselective silylation. **S. Wiskur***

19:30 – 868. Iridium-catalyzed asymmetric hydrogenation of pyridinium salts for constructing multiple stereogenic centers on piperidines. **A. Iimuro**, S. Hida, Y. Kita, K. Mashima*

19:45 – 869. Studies on the asymmetric Meinwald rearrangement of spiro-epoxides: Enantioselective and memory of chirality (MOC) strategies. N. Jeedimala, **S.P. Roche***

20:00 – 870. Catalytic asymmetric hydrogenation of carbocyclic arenes. **R. Kuwano***

20:15 – 871. Ethano-strapped Tröger's base analogs for materials chemistry applications. **A.C. Try***, M. Hashemi Karouei

Hawaii Convention Center
Halls I, II, III

Supramolecular Chemistry at the Interface of Materials, Biology, and Medicine (#300)

Organized by: S. Zimmerman, Z. Li, K. Kim
Presiding: S. Zimmerman

Poster Session
19:00 – 21:00

872. Catch and release of small molecules with porous nanocapsules. **E. Pinkhasik***, S. Dergunov

873. Dendritic single-molecule fluorescent probe that is photostable and minimally blinking. **S.Y. Sang**, S. Zimmerman*

874. Targeting methylated peptides using highly functionalized p-sulfonato calix[4]arenes as a biomimic. **A. Shaurya**, K. Daze, G. Garnett, J. Li, T. Henderson, M. Starke, L. Voss, F. Hof*

875. Synthesis, liquid crystal formation, and double helix-random coil transition in bulk of ethynylhelicene oligomers possessing dendric mesogenic moieties. **N. Saito**, M. Yamaguchi*

876. Engineering of redox metallocenyl nanomaterials. **A. Rapakousiou***, D. Astruc

877. Anti-quorum sensing properties of inclusion complex of *N*-acylhomoserine lactone with alkylamine-modified cyclodextrin. **A. Kamimoto**, S. Ito, N. Kato, T. Ikeda, T. Morohoshi

878. Quorum quenching techniques using modified cyclodextrins. **T. Ikeda**, T. Morohoshi, N. Kato, S. Ito

879. Antibiofilm properties of inclusion complex of *N*-acylhomoserine lactone with cyclodextrin and its derivatives. **T. Azuma***, S. Ochiai, T. Ikeda, T. Morohoshi

880. Influence of molecular weight of humic substances on redox activities. **Z. Yang**, J. Jiang*

881. Cyclodextrin-based switchable DNA condenser. **Y. Chen**, P. Hu, Y. Liu

882. Self-assemble behavior of the stimuli-responsive helical polysaccharide derivatives. **S. Tamari***, S. Shinkai

883. Supramolecular polymer of metal accumulating dendrimer. **S. Mendori***, K. Albrecht, K. Yamamoto

884. Diphenylacetylenes: A versatile platform for molecular switching. **P.C. Knipe***, S. Thompson, A.D. Hamilton

885. Capture and release of guest molecules by reduction-responsive cyclophane oligomers having disulfide linkage.

O. Hayashida*, Y. Nakamura, K. Kojima, K. Nishino, S. Kusano

886. Quartz crystal microbalance analysis of the complex formation of bacterial intercellular signaling molecules with receptors. **H. Sasa**, Y. Takayama, E. Nasuno, K. Iimura, N. Kato*

887. Autoinducer trapping polymers that inhibit bacterial cell-to-cell communication. **N. Kato***, R. Kawakami, C. Okano, Y. Takayama, H. Ozone, K. Iimura, E. Nasuno

888. Supramolecular assembly based on porphyrin and dithienylethene-modified permethyl- β -cyclodextrin. **Y. Zhang**, G. Liu, X. Xu, Y. Liu

889. Rapid access to phospholipid analogs using thiol-yne chemistry. **C. ZHOU***, N.K. Devaraj

890. Synthesis of bis(terpyridyl)anthracene-bridged-di[24]-crown-8 europium(III) complex and its assembly behavior with ferrocene derivative. **H. Zhang**, D. Guo, J. Wang, Y. Liu

891. CB[8]-based fluorescent supramolecular assembly with polymeric rull(II)/tri(bipyridine) centers. **W. Zhang**, Y. Chen, Y. Liu

892. Molecular binding behaviors between pyridinium dyes and water-soluble crown ether. **X. Zhang**, Y. Zhang, Y. Liu

893. Amphiphilic diselenide-containing supramolecular polymers. **Z. Wang**

894. Adhesion between materials using host-guest interaction and covalent bond formation reaction. **T. Sekine**, Y. Takashima, A. Harada*

895. Amide-linked bisureas with stimuli-responsive chloride transport activities. **E. Park***, K. Jeong

Hawaii Convention Center
Halls I, II, III

Fluorinations and Fluoroalkylations (#310)

Organized by: S. Prakash, T. Ritter, K. Mikami, S. Fuster, J. Hu
Presiding: S. Fuster, T. Ritter

Poster Session

19:00 – 21:00

896. Synthesis of 3-fluorinated cyclopropene derivatives and Diels-Alder reactions with 1,3-diphenylisobenzofuran. **G. Lee***, H. Lin, H. Lee, F. Ho

897. Nickel(0)-catalyzed selective co-trimerization or cross-trimerization reactions of ethylene, tetrafluoroethylene, and/or aldehydes. **M. Ohashi***, T. Kawashima, H. Shirataki, K. Kikushima, S. Ogoshi*

898. Synthesis of gem-difluorocycloalkenes via regioselective ring-opening reaction and subsequent RCM reaction using gem-difluorocyclopropanes as starting compounds. **Y. Masuhara***, T. Nokami, T. Itoh

899. Facile synthesis of 2-(perfluoroalkyl)indoles by palladium-catalyzed C-H activation. **D. Shen**, J. Han, J. Chen, H. Zhang, **W. Cao***

900. Copper-catalyzed oxidative cyclization: Synthesis of 3-carbonyl-1-perfluoroalkyl-pyrrol[1,2-a]quinolines. **Z. Xu**, J. Han, J. Chen, H. Zhang, **W. Cao***

901. Efficient synthesis of 2-perfluoroalkyl pyrrole derivatives. **X. Sun**, J. Han, J. Chen, H. Zhang, **W. Cao***

902. Catalytic electrophilic fluorination with hypervalent iodine reagents. **N. Ilchenko***, B. Tasch, K.J. Szabo

903. Fluorous nanochannel constructed by self-assembly of fluorinated macrocycles: Ultrafast water transport. **Y. Itoh***, T. Konda, K. Sato, T. Aida*

904. Fluorination of isoxazoles and its application for the synthesis of 5-hydroxy-4,4-difluoroisoxazolines. **K. Sato***, G. Sandford, S. Akiyama, M.J. Lancashire, Y. Konishi, A. Tarui, M. Omote, A. Ando

905. An efficient generation and its synthetic applications of lithium 4-bromo-3,3,4,4-tetrafluorobutynide. **Y. Watanaabe**, T. Konno*

906. Versatile procedure for fluorocyclization of tryptamines and its application to synthesis of protobutonine A analog. **T. Fujiwara***, Y. Nishimura, H. Yasuda, H. Nambu, T. Yakura*

907. Catalytic introduction of difluoromethyl and difluoromethylene groups with difluorocarbene and its complexes. **K. Fuchibe**, T. Aono, J. Hu, R. Takayama, Y. Koseki, M. Bando, J. Ichikawa

908. Aminotrifluoromethylation via cyclic amine formation of olefins. **S. Kawamura**, H. Egami, M. Sodeoka*

909. Synthesis and crystallographic study of perfluoroalkylated naphtho[2,1-b:6,5-b']dithiophene. **E. Nogami**, T. Yajima*

910. Ring-opening addition reaction of gem-difluorocyclopropane via radical reaction process. **K. Narita**, T. Nokami, T. Itoh

911. De novo synthesis of fluorinated carbohydrate building blocks. **C. Takayanagi**, A. Harada, T. Nokami*, T. Itoh*

912. Copper-catalyzed hydrofluorination of α,β -acetylenic esters and aroylfluorination of epoxides using benzoyl fluoride as fluorine source. **D. Shiozaki**, H. Kuniyasu, M. Nakazaki, T. Iwasaki, N. Kambe

913. Highly diastereoselective synthesis of CF_3 -containing spirooxazolines and spirooxazines by photoredox catalysis. **N. Noto**, T. Koike*, M. Akita*

914. Copper-catalyzed regioselective trifluoromethylthiolation of pyrroles and aryl amines by trifluoromethanesulfonilyl hypervalent iodonium ylide. **Z. Huang**, N. Shibata

915. Catalytic trifluoromethylthiolation of allylsilanes and silyl enol ethers using trifluoromethanesulfonilyl hypervalent iodonium ylide. **S. Arimori**, N. Shibata*

916. Development of electrophilic pentafluorophenylation and pentafluorosulfanylation using diaryliodonium salts. **K. Matsuzaki**, N. Shibata*

917. Synthesis of pentafluorosulfanylphenyl containing heterocycles and their biological activities. **E. Tokunaga***, H. Akiyama, N. Shibata

918. Radiosynthesis of deoxyfluorosucrose analogs and their in vivo study of sucrose transport in maize leaves. **C.S. Hampton**, T. Brossard, D. Rotsch, W. Ying, V. Gaddam, M. Harmata, J. Robertson, M. Swyers, S.S. Jurisson, D.M. Braun

919. Detection of HF by the open-shell P-heterocyclic system. **S. Ito***, Y. Ueta, K. Mikami

920. Organocatalytic enantioselective fluorination of α,α -disubstituted aldehydes. **K. Shibatomi***, K. Kitahara, T. Okimi, S. Iwasa

Hawaii Convention Center
Halls I, II, III

Nanomaterials as Catalysts for Green Chemistry (#313)

Organized by: A. Moores, Y. Uozumi, C. Li, R. Varma

Poster Session

19:00 – 21:00

921. Cobalt-rhodium heterobimetallic nanoparticles as catalysts for the amination of aldehydes and ketones with amines and nitroarenes. **Y. Chung***, J. Park

922. Core-shell nanostructured Au@CeO₂ catalyst for the highly selective semihydrogenation of alkynes to alkenes.

M. Yamamoto, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa, K. Kaneda*

923. Preparation of SiO₂-coated SnPt bimetallic nanoparticle catalysts for selective hydrogenation of unsaturated aldehyde.

K. Tanaka*, T. HARA, T. Imai, A. OKEMOTO, Y. ICHIHASHI, S. NISHIYAMA

924. Development of gallium cation-exchanged montmorillonite catalyst for de-polymerization of polyethers. **S. Yamada**, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa*

925. Complementary catalysis of core-Pd and shell-Ag for selective semihydrogenation of alkynes. **T. Urayama**, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa, K. Kaneda*

926. Transformation of terminal alkenes into primary allylic alcohols over supported Pd catalysts. **Z. Zhang***, T. ISHIDA, H. Murayama, T. Fujitani, M. Tokunaga

927. Microwave-ultrasound simultaneous irradiation: A hybrid technology applied to ring closing metathesis in glycerol micelles. **E. Colacicino**, M. Radou

928. Direct alpha arylation of various ethers with palladium loaded titanium oxide photocatalyst. **a. tyagi***, T. Matsumoto, T. Kato, H. Yoshida

929. Cyanomethylation of alkane by metal loaded titanium dioxide photocatalyst.

E. WADA, T. TAKEUCHI, H. Yoshida*

* Principle Author

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onlineprogram

- 930.** Designing trimodal zeolite catalyst for upgrading the coal-derived fuels. **L. Tan**, C. Xing, G. Yang, Y. Yoneyama, N. Tsubaki*
- 931.** Practical iron-catalyzed oxidation of styrenes and alcohols by hydrogen peroxide. **S. Tanaka**, Y. Kon, k. sato
- 932.** Liquid phase alcohol oxidation reaction using molecular oxygen. **N. Muranaka**, Y. Yoneyama, N. Tsubaki*
- 933.** Catalytic nanostructure and mechanism of $\text{Re}_{0.5}\text{-Pd}/\text{SiO}_2$ for hydrogenation of carboxylic acid. **Y. Takeda**, M. Tamura, Y. Nakagawa, K. Tomishige*
- 934.** Selective 1,4-hydroisilylation of α,β -unsaturated ketones over supported PdAu alloy catalysts. **K. Endo**, H. Miura, T. Shishido
- 935.** Monolithic Pd catalyst for the direct oxidative esterification of methacrolein to methyl methacrylate. **Y. Diao***, P. Feng, S. Zhang
- 936.** Relationship between the atomic-scale structure of Au-Ag bimetallic catalysts and their catalytic performance for 4-nitrophenol reduction as a model reaction. **I.J. Godfrey**, N. Dimitratos, I.P. Parkin, S. Maenosono, G. Sankar*
- 937.** Inhibitory effect to pathogenic bacteria of visible light responsive type nanosilver photocatalyst. **S. Tajiri**, M. Miyazaki, K. Tanaka, K. Ito
- 938.** Kinetic studies of noble metal nanoparticle catalyst microenvironments in water. **A.D. Quast***, I. Zharov, M. Bornstein, J.S. Shumaker-Parry
- 939.** Heterogeneous Lewis acid catalysis with polymeric rare earth alylsulfonates. **P. Tungjirathitikan**, H. Furuno*, J. Inanaga
- 940.** Preparation of montmorillonite-supported late transition metals and catalytic decarbonylation of arene carbdehydes. **T. Moura**, T. ISHIDA, H. Murayama, M. Tokunaga
- 941.** Selective hydrogenation of α,β -unsaturated aldehydes over supported NiPt alloy catalyst. **K. Noguchi**, H. Miura, T. Shishido
- 942.** Characterization of Pd-Ni alloy catalysts for hydrogenolysis of benzyl alcohols. **H. Murayama***, K. Nakamura, T. ISHIDA, T. Honma, H. Ohashi, T. Yokoyama, A. Hamasaki, M. Tokunaga
- 943.** Characterization of supported gold nanoparticle catalysts prepared by impregnation method using amino acid gold complexes as precursors. **T. Hasegawa***, Y. YAMAMOTO, T. ISHIDA, H. Murayama, T. Honma, H. Ohashi, T. Yokoyama, M. Okumura, M. Tokunaga
- 944.** [2+2+1] Cycloaddition of aldehydes, alkynes, and CO by supported Ru catalysts. **H. Miura**, K. Takeuchi, T. Shishido*
- 945.** Development of high-throughput flow system using Ni-Zn mixed based salt catalyst: Application for enone epoxidation with hydrogen peroxide. **A. Hayashi**, T. Hara, N. Ichikuni, S. Shimazu*
- 946.** Chitin-supported ruthenium as a catalyst for nitrile hydration. A. Matsuo, **T. Isogawa**, Y. Morioka, B.R. Knappett, A.E. Wheatley, S. Saito, H. Naka
- 947.** Decarbonylation of furfural catalyzed by zirconia and ceria supported Pd catalysts. **K. Kume**, T. ISHIDA, K. Kinjo, T. Honma, H. Ohashi, T. Yokoyama, H. Murayama, Y. Izawa, M. Utsunomiya, M. Tokunaga
- 948.** Highly ordered polymer as ligand for palladium catalyst. **H. Kim**, H. Lee*
- Hawaii Convention Center
Halls I, II, III
- Organic Solid-State Chemistry: Structure, Property & Reactivity (#398)**
- Organized by: M. Sakamoto, L. MacGillivray, J. Vittal
- Poster Session
19:00 – 21:00
- 949.** Cocrystallization-based control over dichroism in crystalline molecular solids. **O. Bushuyev***, T. Friscic, C. Barrett
- 950.** Multiple photoluminescence of biphenylgold(I)-isocyanide complex: Mechanochromic single crystals including various small organic molecules. **M. Jin***, T. Seki, H. Ito
- 951.** Re-examination of amino acid NCA polymerization 65: Topochemical polymerization of L-glutamic acid ester N-carboxy anhydrides. **H. Kanazawa***, A. Inada
- 952.** Positive phototaxis of oil-droplets comprising of a caged oleic acid against an anisotropic UV irradiation. **K. Suzuki***, N. Nakayama, T. Sugawara*
- 953.** Low-temperature induced phase transition of nitrobenzene derivatives - negative thermal expansion. **H. Takahashi***, T. Nakamura, A. Oyamada, H. Tsue, R. Tamura
- 954.** Family of thermosalient crystals: From serendipity to design. **D. Tan***, J.G. Hernández, T. Friscic
- 955.** Twisting and piezochromism of pi-conjugated molecules using aromatic interactions. **S.W. Thomas***
- 956.** Solid-state recognition and selective binding of organic isomers. **K. Uzarevic***
- 957.** Crystal structures and desolvations of metoclopramide hydrochloride monohydrate and solvates. **Y.P. Nugraha***, O.D. Putra, H. Uekusa
- 958.** Dehydration mechanism of Ciprofloxacin HCl and its implication to physicochemical properties. **OD. Putra**, R. Toyoshima, A. Sekine, H. Uekusa*
- 959.** Magneto-structural correlation in the crystals of *N,N*-bis(*tert*-butylphenyl) nitroxyl radical derivatives. **K. Adachi***, K. Miyamoto, R. Suzuki, Y. Miura, N. Yoshioka
- 960.** Pseudopolymorphic phase transformation of potassium mefenamate hydrate crystal. **A. Egami**, N. Takata, A. Sekine, H. Uekusa
- 961.** Crystal structure change in dehydration of ASP015K hydrobromide hydrate crystals. **N. Hamada**, K. Gao, H. Uekusa
- 962.** Structural motif in itraconazole pharmaceutical co-crystal. **R. Hashimoto**, A. Sekine, H. Uekusa
- 963.** Creation of fluorogenic sensors for aromatic hydrocarbons by supramolecular porous hosts. **S. Hatanoaka**, T. Ono*, Y. Hisaeda
- 964.** Crystal structure and gas adsorption behavior of *N*-protected DL-phenylalanine-glycine. **A. Hisashi***, M. Kochunnoony, R. Tamura, H. Tsue, H. Takahashi
- 965.** Crystal structures of oily medicinal drugs determined by "crystalline sponge method". **M. Kawahata**, T. Akaiishi, Y. Hirose, S. Komagawa, K. Ohara, K. Yamaguchi*
- 966.** Solid-state optical properties and crystal structures of 1,4-dipropoxy-9,10-anthraquinone polymorphs. **C. Kitamura***, S. Li, M. Takebara, Y. Inoue, K. Ono, T. Kawase, K.J. Fujimoto
- 967.** Polymorphism of β -carboline derivatives. **H. Masu**
- 968.** Preparations and crystal structures of diacylene derivatives carrying nicotinic esters. **S. Minami**, I. Iwahashi, T. Okuno*
- 969.** Discovery of the K_4 structure formed by a triangular π radical anion, $\text{NDI}^{\cdot-}$. **A. Mizuno**, Y. Shuku, R. Suizu, M.M. Matsushita, M. Tsuchizui, K. Awaga*
- 970.** Construction of non-interpenetrated hydrogen-bonded hexagonal networks with multiple types of pores based on dehydrobenzo[18]annulene derivative. **S. Nakagawa**, I. HISAKI*, N. TOHNAI, M. MIYATA*
- 971.** Magneto-structural correlation in chromium(V) nitride complexes with salicylideneaniline ligands carrying electron withdrawing group. **S. Nakagome**, Y. Takahashi, Y. Miura, N. Yoshioka
- 972.** Computational search of packing and conformational polymorphs for organic molecules: Crystal structure prediction. **S. OBATA**, H. Goto
- 973.** Dielectric response and structural phase transitions of charge-transfer complex crystals of polar acceptor molecules. **M. Ohtani**, J. Harada*, Y. Takahashi, T. Inabe*
- 974.** Crystal structure and gas adsorption behavior of magnesium porphyrin with open coordination sites. **R. Oketani**, H. Takahashi, R. Tamura, H. Tsue*
- 975.** Inclusion crystals and 1D channel structures using H-shaped CTXP host molecule. **K. Ota***, A. Sekine, H. Uekusa
- 976.** Design of organic ionic crystals showing ferroelectricity from molecular rotation. **H. Oyamaguchi***, T. Shimojo, J. Harada, Y. Takahashi, T. Inabe
- 977.** Supramolecular photochromism of bipyrindinium derivatives appended a crown ether. **R. Satake***, H. Guo, M. Takahashi, T. Kuwabara
- 978.** Variable fluorescence property of diarylmethanoboron difluorides manipulated by crystal packing structure controlled by steric geometry of substituents. **A. Sakai**, E. Ohta, Y. Yoshimoto, Y. Matsui, H. Ikeda
- 979.** Control of solid-state *trans-cis* photoisomerization rate of dual photoreactive complexes. **A. Sekine***, S. Tamari, H. Uekusa
- 980.** CT complexes of unique molecular geometries from pincer-shaped pyrene donors and TCNQ. **Y. Shibusawa**, Y. Itoh*, T. Aida*
- 981.** Novel dual-chromic complex by using salicylideneaniline derivatives. **H. Sugiyama***, A. Sekine, H. Uekusa
- 982.** Emission properties of diarylmethanoboron difluorides controlled by the steric bulkiness of substituents. **M. Tanaka**, A. Sakai, Y. Yoshimoto, Y. Matsui, E. Ohta, K. Mizuno, H. Ikeda*
- 983.** 1D and 2D interaction motif curcumin co-crystal. **K. Teraoka**, A. Sekine, H. Uekusa
- 984.** Negative differential resistance and FET characteristics in TFT-TCNQ at low-temperature. **D. Tonouchi**, M.M. Matsushita, K. Awaga
- 985.** 3D dirac cones in the K_4 crystal. **M. Tsuchizui**
- 986.** Mechanism of photoversible topochemical polymerization via [2+2]-cyclodaddition of thymine derivative in the crystal. **A. Udagawa***, P. Johnston, K. Saito, A. Sakon, R. Toyoshima, H. Uekusa, H. Koshiba, T. ASAHI*
- 987.** Asymmetric synthesis of isoindolinones from achiral materials without an external chiral source. **K. Watanebe**, H. Ishikawa, N. Uemura, F. Yagishita, T. Mino, M. Sakamoto*
- 988.** Asymmetric stereoisomerization of achiral 3,4-diphenylsuccinimides involving dynamic preferential crystallization. **F. Yagishita**, Y. Kunito, Y. Kasashima, T. Mino, M. Sakamoto*
- 989.** Control of molecular arrangement mediated by the interaction between benzene-perfluorobenzene. **R. YAMASAKI***, M. Iida, R. Nagata, A. Ito, A. Tanatani, H. Kagechika, I. Okamoto
- Hawaii Convention Center
Halls I, II, III
- Cognizance of Endangered Elements for Organic Synthesis (#415)**
- Organized by: H. Tsuji, S. Zhu, G. Konishi, C. Luscombe, L. Campeau
- Poster Session
19:00 – 21:00
- 990.** Solvatochromic pyrene analogs of Prodan exhibiting high fluorescence quantum yields and photostability. **S. Agano***, Y. Niko, G. Konishi
- 991.** Functional poly(2-oxazoline)s possessing solvatochromic fluorescent pyrene dye and the development of fluorescent hydrogel. **C. Chen**, G. Konishi
- 992.** Iron-catalyzed diboration and carboboration of alkynes. **T. Hatakeyama**, N. Nakagawa, M. Nakamura
- 993.** 3D assembly of pyrene chromophore on phenolic resin oligomer scaffold enhances fluorescence quantum yield. **K. Kamei***, K. Sumi, G. Konishi
- Hawaii Convention Center
Halls I, II, III
- * Principle Author**
- Photoredox Catalysis in Organic Synthesis (#440)**
- Organized by: D. Nicewicz, S. Fukuzumi, W. Xiao
- Poster Session
19:00 – 21:00
- 1008.** Visible-light initiated oxidative cyclization of phenyl propiolates with sulfinic acids to coumarin derivatives under metal-free conditions. **L. Wang***
- 1009.** Homogeneous and heterogeneous photoredox catalyzed hydroxymethylation of carbonyl compounds. **M. Reckenthaler**, A.G. Griesbeck*

- 1010.** Fluoride salts accelerated visible light-induced alylation of α -halo carbonyl compounds with allyl boron compounds by organic dye catalyst. **N. Esumi**, I. Suzuki*, M. Yasuda
- 1011.** Photoredox of heterocycles in continuous flow. **S. Parisien-Collette**, A. Hernandez-Perez, S. Collins*
- 1012.** Direct coupling of aliphatic carboxylic acids with aryl halides. **R. Evans**, E. Weirin, D. Hager, D. MacMillan
- 1013.** Switching on elusive organometallic mechanisms with photoredox catalysis. **J.A. Terrett**, J. Cuthbertson, V. Shurtliff, D. MacMillan*
- 1014.** Synthesis and chemical properties of pyrimidine-annulated 1-azazulene derivatives: Autorecycling oxidation of some amines under photo-irradiation. **T. Takayasu**, T. Matsuura
- 1015.** Visible light induced photocatalysis for C–H imidation of arenes and heteroarenes. **D. Lee**, H. Kim, T. Kim, S. Roh, D. Lee, C. Lee*
- 1016.** Intermolecular [3+2] annulation of cyclopropanylanes with alkynes, enynes, and dynes via visible light photocatalysis. **T.H. Nguyen**, S. Morris, N. Zheng*
- 1017.** Synthesis of α -linked 2-deoxy glycosides enabled by visible light mediated tin free deiodination. H. Wang, P. Shu, J. Tao, W. Chen, W. Yao, Y. Xu, X. Zhao, Y. Zhao, X. Xiao, Y. Zhu, J. Zeng, Q. Wan*
- 1018.** Photoredox catalyzed [4+2] annulation of cyclobutylanilines and alkynes. **J. Wang**, N. Zheng
- 1019.** Metal-free ring-opening metathesis polymerization. **A.E. Goetz**, K.A. Ogawa, A.J. Boydston
- 1020.** Photocatalytic decarboxylative reduction of carboxylic acids and its application in asymmetric synthesis. **G. Bergonzini**, C. Cassani, C. Wallentin*
- 1021.** Decarboxylative functionalization of β -hydroxy amine acids via photoredox catalysis and its application to the synthesis of the functional 1,2-amino alcohol derivatives. **S. Inuki**, K. Sato, Y. Fujimoto
- 1022.** Visible light-mediated aromatic substitution reactions of cyanoarenes with dihydropyridines via dual carbon–carbon bond cleavage. **S. Nojima***, K. Nakajima, Y. Nishibayashi
- 1023.** Palladium catalyzed radical vinylation of alkyl iodides under photoradiation conditions. **S. Sumino**, I. Ryu*
- 1024.** Homolysis of amide N–H bonds via proton-coupled electron transfer: Development of a catalytic alkene carboamination. **G. Choi**
- 1025.** Regiospecific intermolecular aminohydroxylation of olefins by photoredox catalysis. **K. Miyazawa***, T. Koike, M. Akita
- 1026.** Multistep organic reaction using a glass-milled photocatalytic microchip. **A. Nakamura**, K. Yoshida, S. Amanuma, S. Kuwahara, K. Katayama*
- 1027.** Synthesis of alkyl alkynyl ketones by Pd/light-induced carbonylative Heck reaction of alkyl iodides. S. Sumino, Y. Hamada, T. Uti, T. Fukuyama, I. Ryu*
- 1028.** Highly diastereoselective fused indole-synthesis using visible light. **S.A. Morris**, T.H. Nguyen, N. Zheng*
- 1029.** Universal approach to radical cross-dehydrogenative couplings (CDC) of bromoalkanes to heteroaromatics. **T. McCallum**, L. Barrault*
- 1030.** Metal-free photoredox catalysis for aromatic substitutions. **A. Jacobi von Wangenheim***

Hawaii Convention Center
Halls I, II, III

Catalytic Multicomponent, Tandem and Cascade Reactions (#455)

Organized by: B. Arndtsen,
J. Montgomery, K. Nozaki
Presiding: B. Arndtsen

Poster Session 19:00 – 21:00

- 1031.** Lewis acid-catalyzed cyclization reactions of amides of ethenetricarboxylates. **S. Yamazaki***, M. Niina, K. Ueda

- 1032.** Combined ecofriendly cascade synthesis using combinations of heterogeneous metal/organic catalysts/enzymes. **A. Córdova***, S. Afewerk, C. Carlos-Palo Nieto
- 1033.** Consecutive olefin isomerization hydroformylation with hemilabile tridentate phosphite modified rhodium catalysts. **D. Selet***, C. Kubis, W. Baumann, A. Spannenberg, A. Boerner, R. Franke
- 1034.** Palladium(0) catalyzed one-pot synthesis of 2-substituted indoles. **H. Yamada***
- 1035.** Intramolecular cycloaddition reactions of ethenetricarboxylate derivatives. **S. Yamazaki**, H. Sugiyama, M. Niina
- 1036.** Five-membered ring construction via chain-walking cycloisomerization of various 1,n-dienes catalyzed by palladium complexes. **T. Hamasaki**, F. Kakiuchi, T. Kochi*
- 1037.** Reductive coupling reaction of alkynes, acrylates, and carbon dioxide under cobalt catalysis. **K. Nogi**, T. Fujihara*, J. Terao, Y. Tsuji*
- 1038.** Copper-catalyzed silylative allylation of ketones and aldehydes employing alenes and silylboranes. **T. Yamaguchi**, Y. Tani, T. Fujihara, J. Terao, Y. Tsuji*
- 1039.** Cu^{II}/Rh^I-catalyzed tandem convergent multicomponent reaction for regio- and stereocontrolled synthesis of γ -oxo- β -amino esters. **D. Jung**, H. Jeon, J. Lee, S. Lee*
- 1040.** Chemoselective Reformatsky-Negishi approach to α -haloaryl esters. **X. Linghu***
- 1041.** Modular synthesis of multisubstituted furans through palladium-catalyzed three-component protocol of imines, alkynylodonium reagents, and carboxylic acids. **J. Wu**, N. Yoshikai
- 1042.** Catalytic Friedel-Crafts alkylation/Michaelis-Menten cascade reaction of donor-acceptor cyclopropanes with electron-riched benzenes. **S. Sin**, S. Kim*
- 1043.** Copper-catalyzed double 3-arylation of 3-diazoindolin-2-imines: An efficient strategy to prepare 3,3-diarylindolin-2-imines. **Y. Wang**, P. Lyu
- 1044.** Rhodium-catalyzed enantioselective [2+2+2] cycloadditions of 1,6-enynes with alkenes. **K. Masutomi**, K. Tanaka
- 1045.** Palladium-catalyzed selective olefin isomerization via chain walking. **Y. Yamasaki**, F. Kakiuchi, T. Kochi*
- 1046.** Divergent cascade pathways of the transient palladium complex in palladium-catalyzed intramolecular Heck-type reactions. **J. Lee***, W. Lee, S. Lee*
- 1047.** Synthesis of sila-bicycles by ring-closing diene-yne metathesis reaction. **Y. Nakamura***
- 1048.** Asymmetric synthesis of functionalized 1,4-dihydroquinolines via a one-pot Michael/aza-cyclization domino reaction and dehydration sequence. **H. Kim**, S. Kim*
- 1049.** Palladium-catalyzed (Ullmann-type) reductive homocoupling of the Blaise reaction intermediate. **Z. Xuan**, S. Lee
- 1050.** Cu^{II}/Rh^I-catalyzed tandem convergent synthesis of multifunctionalized amino acid derivatives involving Rh-carbenoid promoted Claisen rearrangement. **M. Kwak**, H. Jeon, S. Lee*
- 1051.** Pd-catalyzed cascade borylative cyclization reactions of polynsaturated compounds. **M.E. Buñuel***, R. López-Durán, A. Martos-Redruejo, V. Pardo-Rodríguez, J. Marco-Martínez, D.J. Cárdenas*
- 1052.** Fe-catalyzed Kumada-type alkyl-alkyl and cascade cyclization-Kumada alkyl-alkyl cross-coupling using NHC ligands. **I.E. Ortín Remón***, N. Cabrera-Lobera, G. Caballero-Santiago, M.E. Buñuel, D.J. Cárdenas
- 1053.** Ruthenium-catalyzed alkylation of barbituric acids with alcohols: A simple, green, and efficient protocol of barbituric acids alkylation. **A.E. Putra**, Y. Oe, T. Ohta*
- 1054.** Palladium-catalyzed three-component reaction of 3-(tributylstannyl)allyl acetates, aldehydes, and organoboranes: A new entry to stereoselective synthesis of (E)-anti-homoallylic alcohols. **M. Sugata**, Y. Horino
- 1055.** Ni-catalyzed dimerizative alkylarylation of 1,3-butadiene by alkyl halides and aryl Grignard reagents. **T. Iwasaki**, A. Fukuoka, H. Kuniyasu, N. Kambe*
- 1056.** Palladium-catalyzed cascade reactions of alkynes with alkenes in ionic liquids. **J. Li**, S. Yang, H. Jiang
- 1057.** Synthesis of quinoline-derived "archipelago model" asphaltene compounds via a multicomponent strategy. **D.E. Scott**, A.T. Iarovoi, R.J. Hamilton, J. Stryker*
- 1058.** Palladium-catalyzed multicomponent reaction of 3-(tributylstannyl)propargyl acetates, aldehydes, and organoboranes. **A. Aimon**, Y. Horino

Thursday Morning

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 2

Reactive Intermediates and Unusual Molecules (#7)

Organized by: R. Sheridan, M. Abe, W. Leigh

- 8:00 – 1059.** Toward synthesis of thermally stable triplet carbenes. **Y. Yamamoto***, J. Yamamoto, S. Fuku-en, K. Furukawa, R. Kishi, M. NAKANO

- 8:25 – 1060.** Mechanisms of carbene additions to strained C–C π bonds. **Z. Yang**, S. Tsuno, E. Dalchand, K.N. Houk, D.C. Merer*

- 8:50 – 1061.** Exploring paramagnetic main group compounds. **T. Augenstein**, J. Harmer, F. Breher*

- 9:15 – 1062.** Can bulky substituents really keep triplet carbene intact? **K. Hirai***

- 9:40 – 1063.** Carbene-stabilized organic radicals with tunable electrochemical properties. **T.W. Hudnall***, C. Deardorff, R.E. Sikma

- 10:00 – 1064.** Controlling carbene reactivity by weak interactions. **P. Costa**, I. Troisién, S. Radhakrishnan, S. Henkel, M. Fernández-Oliva, E. Sanchez-García, W. Sander*

- 10:25 – 1065.** Toward stable triplet vinylcarbenes. **A.D. Gundmundsdóttir***, S.K. Sarkar
- 10:50 – 1066.** Extremely reactive carbenes: Electrophiles and nucleophiles. **R.A. Moss***, L. Wang, H. Cang, K. Krog-Jespersen

- 11:15 – 1067.** Quantum mechanical tunneling reactions of organic reactive intermediates. **H. Inui**, R.J. McMahon*

- 11:40 – 1068.** Photochemistry and spectroscopy of 5-membered heteroarylcarnbenes and isomeric heterocumulenes. **R. Sheridan***, S.A. Varganov, R. Ghimire, S. Lucas

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41)

Organized by: T. Akasaka, F. Wudl, L. Echegoyen, X. Lu, C. Wang
Presiding: H. Imahori, M. Prato

- 8:00 – 1069.** Photofunctional hybrid nanocarbon materials for solar energy conversion. **H. Imahori***

- 8:40 – 1070.** Clickable fullerene scaffolds: Select your application and click. **J. Nierengarten**

- 9:10 – 1071.** Fullerene recognition of chiral phosphorus-containing concave molecule. **M. Yamamura**, T. Nabeshima

- 9:25 – 1072.** In-plane aromaticity in cycloparaphenylen dications: A magnetic circular dichroism and theoretical study. **A. Muranaka***, N. Toriumi, E. Kayahara, S. Yamago*, M. Uchiyama*

- 9:40 – 1073.** Monometallic cyanide clusterfullerene: A novel form of endohedral fullerenes. **S. Yang***

- 10:00 – 1074.** Synthesis of 1D, 2D, 3D molecular nanocarbons. **K. Itami***

- 10:20 – 1075.** Non-HPLC isolation of uncommon metallofullerenes by a new hyphenated approach. **S. Stevenson***

- 10:40 – 1076.** Synthesis of hydroxylated and lithium ion-encapsulated fullerenes. **K. Kokubo***

- 11:00 – 1077.** Properties and growth mechanisms of endohedral fullerenes. **J. Poblet**

- 11:20 – 1078.** Opportunities and challenges of carbon-based nanomaterials. **M. Prato**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Natural Product-based Drug Discovery (#66)

Organized by: B. Baker, R. Kerr, Y. Qin, D. Uemura, B. Littlefield
Presiding: B. Baker, W. Gerwick, M. Ueda

8:00 Opening Remark

- 8:05 – 1079.** Epigenetic approach to drug discovery of anti-infective fungal metabolites. **D. Demers**, M. Knestrick, R. Fleeman, C. Witowski, B. Vesely, A. Azhari, C. Rice, B. Colon, A. Souza, L. Shaw, D.E. Kyle, **B. Baker***

- 8:45 – 1080.** Aligning bacterial physiology and ecology with drug discovery. **J. Clardy**, E. Mevers, D. Dietrich, E. Hobert, A. Cantley

- 9:25 – 1081.** Chemical biology of coronatine: Pathogenic infection in plants. **M. Ueda***

- 10:00 – 1082.** Discovery and development of anticancer lead compounds from marine cyanobacteria. **W. Gerwick**, J. Almaliti, J. Lee, B. Miller, A. Pereira

- 10:30 – 1083.** Nanomole-scale tools for drug-lead discovery from marine natural products. **T.F. Molinski***

- 11:00 – 1084.** Isolation, structure determination, synthesis, and biological characterization of novel bioactive natural products from marine cyanobacteria. **H. Luesch**

- 11:30 – 1085.** New highly stable tricyclic antitubercular ozonides derived from artemisinin. **S. Chaudhary**, P. Jaiswal, V. Sharma, A. Gaikwad, S. Sinha, V. Chaturvedi, Y. Manju, S. Puri, A. Sharon, P. Maulik

- 11:40 – 1086.** Bioorganic studies on the key natural products from venomous mammals. **M. Kita***

- 11:50 – 1087.** Yoshinone A: A novel natural product that shows an anti-obesity activity. **Y. Kawazoe**, T. Koyama, A. Iwasaki, O. Ohno, K. Suenaga, D. Uemura*

Hawaii Convention Center
Halls I, II, III

Molecular and Supramolecular Photochemistry (#71)

Organized by: J. Sivaguru, W. Chung, C. Bohne, c. Tung, M. Sakamoto, V. Ramamurthy

Presiding: C. Bohne, W. Chung, S. Jayaraman, V. Ramamurthy, M. Sakamoto, C. Tung

Poster Session

10:00 – 12:00

- 1088.** Artificial photosynthesis dendrimers integrating light-harvesting, electron delivery, and hydrogen production. **Y. Zeng**, Z. Xun, Y. Li*

- 1089.** Controlled self-assembly pathways by photocyclized product of stilbene dyad. **M. Yamauchi**, S. Yagai*

* Principle Author

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onlineprogram

- 1090.** Photoreactions of amino acid derivatives bearing aromatic group with 1,4-dicyanophthalene. **M. Yamawaki**, Y. Yoshimi*
- 1091.** Decarboxylative radical addition of amino acids to N-acryloyl amino acids via photoinduced electron transfer. K. Osaka, **Y. Yoshimi**
- 1092.** Supramolecular asymmetric photocogenesis mediated by synthetic antibody: Ground- and excited-states interaction studies of synthetic antibody with 2-anthracenecarboxylate. **W. Yospanya**, S. SAKAMOTO, Y. Araki, M. Nishijima, Y. Inoue, T. Wada
- 1093.** Multichromic supramolecular dye architectures for advanced light-harvesting applications. **M. Yousaf**, B.D. Koivisto*
- 1094.** Azobenzene-incorporated BINOLs as stimuli-responsive catalysts. **S. AKURA**, Y. TSUTSUI, M. Uchiyama, K. TAKAISHI, T. Imahori*
- 1095.** Mechanistic investigation of dehydrogenation and deamination in photochemical formation of quinone methides. **N. Basaric***, D. Skalamera, K. Milanic-Majerski, H. Vancik, P. Wan
- 1096.** Two-photon triggered photolabile protecting groups: From molecular engineering to nanostructuration. **F. Bolze**, P. Sebastian, A. Specht, A. Losonczy
- 1097.** Integrating azobenzene into macromolecular metal complexes to generate optical active materials. **S.C. Burdette***, J. Yan
- 1098.** Light induced molecular machine: Ru-thiocene-based supramolecular crystals. **K. Chen***, M. Horie
- 1099.** Light-driven nanofiber and nanoring morphological transformation in an organogel based on an azo bridged bis[azobis[4]arenene]. **P. Su**, K. Chang*, W. Chung*
- 1100.** Spatially directed electron and energy transport in terpyridine based coordination oligomers: A spectroscopic study. **B. Dietzek***
- 1101.** Conjugating artemisinin derivatives with synthetic components for pharmaceutical applications. **A. Eske**, A.G. Griesbeck*, S. Sillner
- 1102.** Controlling energy and electron flow using an organic cavity and an inorganic layered material. **T. Fujimura**, E. Ramasamy, Y. Ishida, T. Shimada, S. Takagi*, V. Ramanurthy*
- 1103.** Laser photolysis studies of triplet sensitization triggered α -cleavage in aromatic carbonyls containing five-membered rings. **S. Fujino**, M. Yamaji*
- 1104.** Solvent and substituent effect on lifetime of colored form of dinitrobenzylpyridine derivatives. **S. Fukuyoshi**, T. Nakayoshi, Y. Watanabe, A. Oda
- 1105.** Photochemical reactions and photophysical properties of dinaphthyrindineamino derivatives. **R. Hagiwara**, S. Karasawa*, N. Koga*
- 1106.** Photochromism and photomechanical bending of diisopropylbenzophenone crystals. **Y. Hagiwara***, M. Kitajima, H. Koshiba, T. ASAIH
- 1107.** Dye-sensitized solar cell of a non-carboxylated dye compound containing cyclodextrin layer. **M. Hara**, T. Takeshita, Y. Kasaba
- 1108.** Photo and thermally induced phase transition of ferrocene-containing rotaxane crystals. **M. Horie***, K. Chen
- 1109.** Laser photolysis studies of photo-induced ω -bond dissociation in aromatic carbonyls having C-C triple bond. **A. Horimoto**, K. Nozaki, M. Yamaji*
- 1110.** Design and synthesis of new caged calcium with high two-photon absorption character. **S. Jakkampudi***, M. Abe, R. Takagi, C. Katan
- 1111.** Completing the cycle: Sustainable, renewable, and recyclable polymers/oligomers derived from biomass through programmed photodegradation. R. Raghunathan, R. Krishnan, R. Saravanakumar, M.P. Sibi, D. Webster, **S. Jayaraman**

- 1112.** Characteristic photoinduced macroscopic dynamics of molecule-based assemblies: Propelling and self-oscillation. **Y. Kageyama***, Y. Kurokome, T. Ikegami, S. Takeda
- 1113.** Amino acid based fluorescent chemosensor for CO₂ using intramolecular hydrogen bonding stabilization: Application to screen relative activities of CO₂ absorbents. **S. Kang**, M. Eom, T. Lim, M. Han*
- 1114.** Photoreaction of push-pull type diquinolinylamine derivatives and alteration of emission and morphology in solution. **S. Karasawa***, J. Todo, K. Usui, H. Suemune, N. Koga*
- 1115.** Synthesis and function of a DNA cleaving molecule possessing phototriggering functionality via a Norrish type II reaction. S. Ueta, F. Yagishita, M. Nishiuchi, **Y. Kawamura***
- 1116.** Photoxxygenation of model compounds for carotenoids. **M. Kleczka**, A.G. Griesbeck, A. de Kiff
- 1117.** Development of new photolabile protecting groups with two-photon absorption ability for physiological studies. **N. Komori**, M. Abe, C. Katan, K. Kamada, K. Furukawa
- 1118.** Photochemistry of N-substituted heteroaromatic salts. **W. Kramer**, C. Mullins, M. Solomon, L. Hoth, A. Allred, E. Stewart, W. Curry
- 1119.** Chiral binaphthyl-tethered azobenzene bis(fattyalcohol) as a chirality switching catalyst. **T. Kuroda**, T. OMAGARI, S. UTO, S. Kurihara, K. TAKAISHI, M. Uchiyama, T. Imahori
- 120.** Photophysical property switching of artificial light-harvesting porphyrin dendrimers in response to monomeric porphyrin guest binding. **H. Lee**, Y. Jeong*, W. Jang
- 121.** Ultra-low power photon upconversion in light-harvesting chromophore arrays. **P. Mahato**, N. Yanai*, N. Kimizuka*
- 122.** Analysis of "excited state C-C bond cleavage-luminescence" phenomenon of methylenecyclopropanes by using laser flash photolysis. **Y. Matsui**, T. Kido, E. Ohita, H. Ikeda*
- 123.** Emission properties of pyrene probes and ring stacking modes on the surface of flexible proteins. **T. Matsuo***, A. Fujii, S. Hirota, H. Matsumura, W. Chung
- 124.** Photoinduced switching to metallic states in 2D organic charge-transfer complex dimethylphenazine-tetrafluorotetraacyanoquinoxidimethane with anisotropic molecular stacks. **H. Matsuzaki***, M. Okura, Y. Ishige, Y. Nogami, H. Okamoto
- 125.** Reversible electronic energy transfer involving supramolecular assemblies and organic-inorganic hybrids. S.A. Denisov, G. Jonusauskas, A. Tron, **N.D. McClenaghan***
- 126.** Photochemistry of pyromellitic diimides. **S. Molitor**, W. Kramer, A.G. Griesbeck*
- 127.** Highly enantioselective biocatalytic enantiodifferentiating photocyclodimerization of 2,6-anthracenedicarboxylate mediated by human serum albumin. **M. Nishijima***, K. Tanaka, G. Fukuhara, T. Mori, Y. Inoue*
- 128.** Highly concentrated millimeter sized domain of lysozyme clusters by laser trapping. **S. Nishimura***, H. Yoshikawa, S. Nakabayashi, K. Yuyama, T. Sugiyama, H. Masuhara
- 129.** Enantioselective photoreactions controlled by the functional group of chiral templates. **Y. Nishiyama***, Y. Suzuki, Y. Yanagisawa, K. Kakuchi
- 130.** Photophysical studies of photoredox catalyzed trifluoromethylation of heteroarenes. **J. Ochola***, M.O. Wolf
- 131.** Identification of photodegradation products of 4,5-dimethoxy-2-nitrobenzyl esters and carbamates having alkyl group at α -position. **N. Okamura**, Y. Saito, T. Kikuchi, K. Shoda, N. Chikaraishi, K. Yamaguchi*
- 132.** Synthesis of fluorescent solvatochromic dyes based on 2-pyridylthiophene compound and tuning of absorption and emission wavelengths by coordination at the pyridyl nitrogen. **Y. Otsuka***, K. Yamada, S. Sakurai
- 133.** Highly selective turn-on near-infrared fluorescent sensor for imaging hydrogen sulfide in living cells. **C. Park**, T. Ha, C. Lee
- 134.** Photochemical behaviors of cationic cyanine dyes on a clay nanosheet. **N. Sato**, T. Fujimura, T. Shimada, S. Takagi*
- 135.** Photoreaction of exo-2,3-diphenyl-6,6-dicyanofulvene dimer. **T. SEGAWA***, T. YAHAJI, H. HONMA, S. SEKIMOTO
- 136.** Photochemical processes of halogenated 1,3-diketone derivatives studied by stationary, single and double laser photolyses. **Y. Suwa**, M. Yamaji*
- 137.** Surface-fixation induced emission of cationic dyes on an anionic clay surface. **D. Tokieda**, N. Sato, T. Fujimura, T. Shimada, S. Takagi
- 138.** Ketoprofen as photoinitiator for anionic polymerization. **Y. Wang***, P. Wan
- 139.** Pyridinium salts as electron traps: An ultrafast transient absorption spectroscopy study. **R.M. Wilson***, I. Khubaibullin, S. Matveev, A.E. Shamaev, A.S. Mereshchenko, K. Karabaeva, M.S. Panov, A.N. Tarnovsky
- Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2
- Molecular Containers (#99)**
- Organized by:* S. Mitsuhashi, L. Isaacs, H. Yang
Presiding: S. Goldup, H. Yang
- 8:00 opening**
- 8:05 – 1140.** Recognition and catalysis in deep cavitations. **J. Rebek**
- 8:35 – 1141.** Molecular self-sorting for controllable suprapolymerization. **X. Zhang**
- 9:05 – 1142.** Metal-ligand assembly using T-shaped, right-angled ligands. **P. Rowsell**, K. Zhu, I. Elgaria, **S. Loeb***
- 9:30 – 1143.** Container molecules for xenon (and other gas) complexation. **K.T. Holman**
- 9:50 coffee break**
- 10:00 – 1144.** Elaborate molecular inclusion methods in metallo-hosts via multipoint noncovalent interactions. **M. Shionoya***
- 10:30 – 1145.** Metallo-cages from cyclotriferratrylene-type ligands. **M. Hardie***, J.J. Henkelis, F. Thorp-Greenwood, T. Ronson, J. Fisher, V.E. Pritchard, N. Cookson
- 10:55 – 1146.** Unimolecular tubular artificial transmembrane channels. **J. Hou**
- 11:20 – 1147.** AllostERIC modulation of supramolecular catalysis in synthetic super-containers. **Z.R. Wang**
- 11:40 – 1148.** Aminocarbohydrates recognition with cucurbit[7]uril. Y. Jang, **Y. Ko**, J. Koo, J. Kchedkar, J. Wang, Y. Rhee, K. Kim*
- Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1
- Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100)**
- Organized by:* D. Hall, B. Wang, P. Duggan, M. Sugino
Presiding: D. Hall
- 8:00 – 1149.** Boron-based anticancer prodrugs that target tumor cells under oxidative stress. **X. Peng***
- 8:30 – 1150.** Boron containing retinoids are potential therapeutic agents for treatment of Alzheimer's diseases. **B.C. Das***, T. Evans
- 8:50 – 1151.** Boronic acid facilitated "click-like" reaction allowing for secondary functionalization. **A. Draganov**, K. Wang, J. Holmes, K. Damera, D. Wang, C. Dai, B. Wang*
- 9:10 – 1152.** Fifth element in drug design: Boron in medicinal chemistry. **L. Rendina***, M. Kassiou, C. Austin, F. Issa, J. Kahlert, R. Narlawar, S. Wilkinson
- 9:40 – 1153.** Saccharide recognition with peptide boronic acids. **P. Duggan***, W. Kowalczyk, D. Haylock, O. Hutt
- 10:00 Break**
- 10:10 – 1154.** Branched peptide boronic acids: Molecular recognition of folded HIV-1 RNA structures. **W.L. Santos**
- 10:40 – 1155.** Boronic acid probes in supramolecular analytical chemistry. **A. Schiller***
- 11:00 – 1156.** DNA modifications with the boronic acid moiety. **B. Wang**
- 11:20 – 1157.** Novel benzoxaboroles as anti-parasitic agents: Discovery and development of new treatments for kinetoplastid diseases. **R.T. Jacobs**
- Hilton Hawaiian Village
Rainbow Tower, Rainbow 1
- Electrochemical Reactions and Mechanisms in Organic Chemistry (#104)**
- Organized by:* K. Chiba, S. Suga, K. Moeller, C. Frontana
Presiding: K. Chiba, K.D. Moeller, D.G. Peters
- 8:00 – 1158.** Examples of redox chemistry conducted in the absence of a traditional supporting electrolyte: Development and use of a composite dispersion. **D. Little***, S.J. Yoo, S. Herold
- 8:15 – 1159.** Electrochemical glycosylation as an enabling tool for oligosaccharide synthesis. **T. Nakami***, Y. Isoda, N. Sasaki, S. Hayase, T. Itoh, R. Hayashi, A. Shimizu, J. Yoshida
- 8:30 – 1160.** Redox and electron mediation behavior of pyridinium ionic liquids and their application to organic synthesis. **H. Shimakoshi***, N. Houfuku, Y. Hisaeda
- 8:45 – 1161.** Electrocatalysis of azobenzene isomerization. **S.C. Blackstock***, C. Saint-Louis
- 9:00 – 1162.** Transition metal free C-C bond formation of brominated 2,2'-biphenyls. **R. Obata***, S. Ohba, Y. Einaga, S. Nishiyama
- 9:15 Break**
- 9:30 – 1163.** Structure-activity relationship of AMP-luciferin analogs for in vivo imaging. **N. Kitada**, S. Iwano, T. Hirano, H. Niwa, S. Maki
- 9:45 – 1164.** Electrochemical reduction of haloacetic acids with sonication at a silver cathode. **E.T. Martin***, D.G. Peters
- 10:00 – 1165.** Synthesis of oxazoline from unsaturated amides using an electrochemically generated ArS(ArSSAr)⁺ pool. **Y. Miyamoto**, K. Matsumoto*, S. Suga, S. Kashimura, J. Yoshida*
- 10:15 – 1166.** EPR and UV-Vis spectroelectrochemical investigations of s-tetrazine derivatives. **M. Lapkowski***, S. Pluczky, P. Zassowski, P. Audebert
- 10:30 Break**
- 10:45 – 1167.** AC-bipolar electrolysis for template-free synthesis of conductive polymer fiber networks. **Y. Koizumi***, H. Nishiyama, I. Tomita, S. Inagi
- 11:00 – 1168.** Reduction of dodecachloropentacyclo[5.3.0.0^{2,6}.0^{3,9}.0^{4,8}]decane (mirex) at silver cathodes assisted by ultrasound. **C.M. McGuire***, D.G. Peters

* Principle Author

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- 11:15 – 1169.** Reductive carboxylation of benzoic acid esters by electron transfer from magnesium metal. **H. MAEKAWA***, H. Okawara, T. Murakami
11:30 – 1170. Global and local chemical descriptors and its use for describing electron transfer events coupled with proton transfer. **C.E. Frontana***

Hilton Hawaiian Village
 Mid-Pacific Center, Coral 4

Recent Trends in Organocatalysis (#122)

- Organized by:* M. Terada, M. Shi, J. Antilla, K. Maruoka
Presiding: K. Ishihara, T. Kawabata, T.H. Lambert, M. Terada
- 8:00 – 1171.** Enantioselective bifunctional N-heterocyclic carbene catalysis. **S. Ye***
8:30 – 1172. Enantioselective iodocyclization induced by chiral base-acid cooperative catalysis. **K. Ishihara***, H. Nakatsuji
9:00 – 1173. Aromatic ions for the design of new organocatalysts. **T.H. Lambert***
9:30 – 1174. Cooperative organocatalysis strategies for synthesis. **K. Scheidt***
10:00 – 1175. Enantioselective synthesis of tetralone-derived natural products based on organocatalytic oxidative kinetic resolution. **K. Nagasawa***
10:30 – 1176. Amino acid-based chiral phosphines for enantioselective nucleophilic catalysis. **Y. Lu***
11:00 – 1177. Enantio- and site-selective molecular engineering by organocatalysis. **T. Kawabata***
11:30 – 1178. Asymmetric counteranion directed catalysis (ACDC): A general approach to enantioselective synthesis.
B. List

Hilton Hawaiian Village
 Mid-Pacific Center, Coral 5

Homogeneous Gold Catalysis: Methods, Theories and Applications (#192)

- Organized by:* L. Zhang, H. Ohno, R. Liu
Presiding: L. Ye
- 8:00 – 1179.** Development of highly effective polymerization processes catalyzed by gold complexes. **F. Nzulu***, J. Goddard, C. Ollivier, L. Fensterbank
8:20 – 1180. Triazole-Au(I) complexes in promoting homogeneous gold catalysis: From stability to selectivity. **X. Shi**
8:50 – 1181. Low-coordinated phosphines for the activation-free LAuCl catalysis. **S. Ito***
9:10 – 1182. Homogeneous gold catalysis vs. heterogeneous gold nanopore, Au-N-Pore, catalysis: Advantages and disadvantages. **Y. Yamamoto**
9:45 break
10:00 – 1183. NHC-AuCl>Selectfluor: A highly efficient catalytic system for the activation of enynes/enynes. **S. Zhu**
10:20 – 1184. Reactivity of gold-cyanomethyl complexes. **S.P. Nolan**, A. Collado, D. Gasperini, D. Cordes, A. Slawin
10:50 – 1185. Discovery of antiresistance agents using gold catalysis. **X. Wang***
11:10 – 1186. Efficient gold catalysis enabled by novel ligands. **L. Zhang***
11:40 – 1187. Gold-catalysed cross-coupling of arenes via double C–H activation. **N. Ahlsten**, X.C. Cambeiro, I. Larrosa*

Hawaii Convention Center
 Halls I, II, III

Molecular Function of Natural Products: Advances towards Chemical Biology (#237)

- Organized by:* M. Ueda, B. Miller, K. Irie, B. Miller, B. Miller, C. Lin, T. Oishi, C. Forsyth, H. Lee
Poster Session
10:00 – 12:00
- 1188.** Crystal structure of *D,L*-racemic supramolecular rare sugars. **T. Senoo**, T. Ishii*, T. Kamakura, M. Mimura, K. Fukada, A. Yoshihara, T. Kozakai, G. Sakane

- 1189.** Discovery of a potent and selective agonist of TRPA1 and direct observation of its binding to TRPA1 by electron microscopy. **J. Takaya**, K. Mio, Y. Mori, M. Uesugi*
1190. Studies toward the total synthesis of amphidinolide N. **Y. Kawashima**, H. Fuwa, M. Sasaki*
1191. Structural insight into the inhibitory mechanism of amyloid β 42 aggregation by non-catechol-type flavonoids. **M. Hanaki**, K. Murakami, K. Akagi, K. Irie*
1192. Jasmonic acid transporter suppresses the excess wounding response in undamaged parts. **Y. Ishimaru**, T. Oikawa, T. Suzuki, H. Matsuda, K. Takahashi, S. Hamamoto, N. Uozumi, T. Shimizu, M. Seo, H. Ohta, M. Ueda*
1193. Oxidative stress-related substance, acrolein, regulates biosystems by reacting with polyamines. **A. Tsutsui***, T. Zako, Y. Yamaguchi, T. Bu, R. Imanaka, S. Kitazume, N. Taniguchi, M. Maeda, K. Tanaka*
1194. Development of the strategy for the selective chemical modification in a hydrophobic site in DNA or RNA. N. Sato, Y. Sasaki, K. Onizuka, K. Yamada, **F. Nagatsugi**
1195. Mechanism for the antibacterial action of epigallocatechin gallate (EGCg) on *Bacillus subtilis*. **A. Horuchi**, J. Sato, K. Shimatani, T. Ozawa, N. Shigemune, D. Tomiyama, T. Sonoda, M. Nakayama, M. Hasumi, T. Miyamoto
1196. In vivo production of eight-membered heterocycles from acrolein and transformation to 3-formyl-3,4-dihydroperipiperidine (FDP). **T. Masayuki**, F. Koichi, K. Tanaka*
1197. Evaluation of the binding site of aplyronine A on tubulin by genetic approach. **K. Yamagishi**, K. Tsuchiya, T. Chinen, T. Usui, M. Kita, H. Kigoshi
1198. Development of novel fluorescent PPI detection system for subtype selective ligand of phytohormone co-receptor. **Y. Takaoka**, M. Iwahashi, T. Iwashita, T. Suzuki, K. Hayashi, S. Egoshi, Y. Ishimaru, M. Ueda*
1199. Development of the new firefly luciferin analog aiming at detection of a free radical in the living body. **S. Ioka***, T. Saitoh, S. Iwano, S. Maki, H. Niwa, M. Imoto, S. Nishiyama
1200. Directed evolution of antibody-like peptides for proteomics. **T. Kawakami***
1201. Glycolipozyme MPase functions as membrane protein integrase *in vivo*. **K. Sawasato***, M. Moser, R. Sato, K. Nishiyama
1202. Reconstitution of glycolipozyme MPase-dependent protein integration into membrane. **M. Sasaki***, H. Matsabayashi, Y. Kuruma, T. Ueda, K. Nishiyama
1203. Characterization of an MPase homologue in plants that catalyzes membrane protein integration. **Y. Endo***, T. Yamaguchi, H. Matsabayashi, Y. Kuruma, T. Ueda, K. Shimamoto, K. Nishiyama
1204. Cell differentiation inducing metabolites from marine sponges. **S. Matsunaga***
1205. Establishment of a 3D cell culture-based screening platform to identify natural products that can regulate trans-epithelial water transport of the human gastrointestinal tract. **S. Fujii**, R. Okamoto*, T. Nakata, K. Suzuki, F. Ishibashi, A. Kawamoto, S.O. Segawa, T. Mizutani, K. Tsuchiya, T. Nakamura, M. Watanabe
1206. Theoretical study on the electronic structure of trimethylamine N-oxide (TMAO) in aqueous solution. **Y. Watanabe**, D. Akase, M. Aida*
1207. Identification of biosynthetic enzymes for MPase, a glycolipozyme essential for membrane protein integration. **R. Sato***, K. Shimamoto, T. Yamaguchi, M. Moser, K. Nishiyama
1208. Extraction of flavor compounds from lemongrass utilizing ionic liquids. **C. Murata**, T. Usuki*
1209. Potent antibacterial compound is isolated from garlic peel. **H. KITAHARA***, A. Ito
- 1210.** Suppression of siRNA off-target effect by chemical modifications which regulate thermodynamics in nucleotide base-pairing. **K. Ui-Tei***, H. Iribe, T. Takahashi
1211. Elucidation for biopactivity of ouabagenin, a presumed endogenous ligand for nuclear receptor. **S. TAMURA**, H. Oishi, T. Abe, M. Okada, M. Ueda
1212. Exploring an appropriate ligand-binding pose by ensemble-based docking. **H. Saito***, K. Kawaguchi, H. Nagao
1213. Mitotic role of estrogen receptor alpha: Stimulation of E3 ubiquitin ligase activity ofUBE3C that facilitates cell proliferation. **M. Okada***, T. Ohta
1214. Voltage-dependent, slowly activated K⁺ channel involved in nyctinasty of *Samanea saman*. **T. Oikawa***, T. Suzuki, Y. Ishimaru, S. Hamamoto, S. Munemasa, Y. Murata, N. Uozumi, M. Ueda
1215. Molecular target of yessotoxin. **N. Matsumori**, H. Tsuchikawa, T. Usui, N. Sugiyama, M. Satake, K. Tachibana
1216. Biological characterization of MetE as a receptor candidate in *Cassia obtusifolia* for the leaf opening factor. **N. Kanzawa***, J. Nishiya, Y. Otsuka, Y. Ishimaru, M. Ueda
1217. Development of small molecular calcium indicators for plant cell. **M. Shigenaga**, M. Imai, Y. Nukadzuka, Y. Takaoka, M. Ueda*
1218. Regulatory mechanism of TRP channel in yeast tonoplast. **S. Hamamoto**, I. Yabe, N. Uozumi
1219. Elucidation of the molecular mechanisms of action of bioactive natural products using high performance affinity beads. **S. Sakamoto**, Y. Yamaguchi, T. Ito, H. Handa*
1220. Molecular mechanism of action of fusocin-based antitumor agents. **J. Ohkanda***, S. Sato, P. Parvatkar, M. Uesugi, N. Kato
1221. Target identification of agelasine D, a marine spongean diterpenoid alkaloid, as an antimicrobial mycobacterial substance. **M. Arai**, Y. Yamano, A. Setiawan, M. Kobayashi*
1222. NMR analysis of ligand-induced structural changes to identify key structures of ligand molecules. **H. Takahashi**
1223. Method for selective clearance of cytosolic proteins via autophagy. **D. Takahashi**, H. Arimoto*
1224. Development of novel protein labeling method useful for plant chemical biology. **Y. Nukadzuka**, Y. Takaoka, M. Ueda*
1225. Acceleration of lipid degradation by widdrol in fully differentiated 3T3-L1 cells. **H. Jeong**, H. Yun, S. Choi, Y. Son, I. Jeong, S. Nam, S. Kim, M. Ham, N. Kim, S. Jin, B. Kim, E. Lee, H. Kwon*
1226. Development of transgenic *Daphnia* for monitoring hormonal activities of chemicals. **Y. Kato**, T. Nakanishi, T. Matsuura, **H. Watanabe***
1227. Development of biactivity-controlled molecular probe to reveal the mechanism of stomatal reopening caused by phytotoxin coronatine. **T. Iwashita**, Y. Takaoka, T. Suzuki, R. Tashita, S. Egoshi, Y. Ishimaru, M. Ueda*
1228. Development of molecular probes based on the partial structure of Amphidinolide 3. **Y. Takeda***, M. Ebine, T. Oishi
1229. Fluorescence-labeled lipopeptides as molecular probes for TLR2. **Y. Arii**, Y. Kawahara, K. Yokoyama, S. Inuki, K. Kabayama, F. Koichi, Y. Fujimoto
1230. Synthesis of desmosine-d₄ for LC-MS/MS analysis in elastin degradation. **D. Watanabe**, T. Usuki*
1231. Study on the novel chemical probes to analyze protein-ligand interactions. **K. Yoneda***, Y. Hu, M. Kita, H. Kigoshi
1232. Natural product-inspired glutamate analogs: The diverted synthesis and the neuronal activity. **M. Chiba**, C. Fujimoto, Y. Ishikawa, M. Oikawa*
1233. In vivo Raman imaging in living guard cells for elucidating the localization of the plant toxin coronatine. **S. Egoshi**, K. Dodo, Y. Ishimaru, T. Iwashita, T. Suzuki, Y. Takaoka, M. Sodeoka, M. Ueda
1234. Design and synthesis of a photoreactive OSW-1 analog and its application to a photoaffinity labeling study. **R. Yamada**, T. Takeshita, M. Hiraizumi, K. Sakurai*
1235. Synthesis of photoreactive O-benzyl-D-serine derivatives for photoaffinity labeling. **T. Yoshida***, Y. Hashidoko, M. Hashimoto
1236. Design and synthesis of a biochemical probe of (+)-macrospheleide A. **J. Sim**, C. Lim, S. Lee, Y. Suh*
1237. Design, synthesis, and biological evaluation of cyclic depsipeptides as chemical probes for study of the tumor microenvironment. **K. Hattori**, K. Koike, K. Okuda, T. Hirayama, H.K. Nagasawa
1238. [¹³C₃, ¹⁵N₁]-labeled isodesmosine, a potential internal standard for the LC-MS/MS analysis in elastin degradation. **T. Tanigawa**, T. Usuki*
1239. Search for Notch signaling inhibitors from natural products. **M.A. Arai***, R. Akamine, R. Okamoto, T. Koyano, T. Kowithayakorn, S.K. Sadhu, F. Ahmed, M. Ishibashi*
1240. Phenol compounds treated cotton and wool fabrics for developing multifunctional clothing materials. **K. Hong***
1241. Host factors enhance antimicrobial activity of "Lysocin E". **H. Hamamoto**, S. Jie, A. Paudel, K. Ishii, J. Yasukawa, K. Sekimizu
1242. Rapid search for naturally occurring neural stem cells activators using stem cell transcription factor Hes1 beads. **M.A. Arai**, N. Ishikawa, T. Kowithayakorn, M. Ishibashi*
1243. Identification of licopyranocoumarin and glycyrrulol from herbal medicines as neuroprotective compounds for Parkinson's disease. **M. Imoto***, T. Fujimaki, S. Saiki, E. Tashiro, D. Yamada, N. Hattori
1244. *Aspergillus kawachii* treatment enhances antioxidative effect of mistletoe through increase in phenolic compound contents. **S. Kim**, **J. Lee**, E. Choi, J. An, J. Moon, S. Kim, K. Song*
1245. Isolation of Notch inhibitors from *Calotropis gigantea*. **T. Yoneyama***, M.A. Arai, R. Okamoto, S.K. Sadhu, F. Ahmed, M. Ishibashi
1246. Isolation and biological activities of novel androgen receptor antagonist produced by Streptomyces. **S. Saito**, T. Fujimaki, E. Tashiro, Y. Igarashi*, M. Imoto
1247. Vascular protective activity of plant-derived caffeoyl quinic acids against HMGBl-induced inflammatory responses. **N. Tuan**, I. Park, E. Lim, H. Kang, B. Jung, J. Bae*, M. Na*
1248. Extraction of citral from lemon myrtle utilizing ionic liquids. **K. Munakata**, T. Usuki*
1249. Widdrol, a sesquiterpene isolated from *Juniperus chinensis*, inhibits angiogenesis and tumor growth by targeting vascular endothelial growth factor receptor 2 signaling. **S. Jin**, H. Yun, H. Jeong, Y. Oh, H. Park, B. Kim, H. Kwon*
1250. Anticancer activity of *Endlicheria anomala* extract by apoptosis induction in human lung and liver cancer cells. **H. Park**, **S. Jin**, Y. Oh, H. Jeong, H. Kwon, B. Kim*
1251. Synthetic studies on funiculosin. **K. Sato**, S. Inuki, Y. Fujimoto

*** Principle Author**

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TECHNICAL PROGRAM

- 1252.** Synthesis of the photoactive phenyl-thiocarbamide derivatives for gustatory receptors elucidation. **A. Ishida***, Y. Hashidoko, M. Hashimoto
- 1253.** Synthetic studies of protoaculeine B. **H. Sugahara**, K. Otsuka, Y. Ishikawa, M. Okawa*
- 1254.** Synthetic study and target analysis of dictyoceratin-A and -C, hypoxia-selective growth inhibitors from marine sponge. **N. Kotoku***, Y. Sumii, T. Kawachi, A. Fukuda, M. Arai, M. Kobayashi*
- 1255.** Synthesis and properties of deuterated cyclo-DOPA derivatives. **S. Nakagawa***, Y. Hashidoko, M. Hashimoto
- 1256.** Formal C-H azidation-based shortcut to diazido building blocks for the versatile preparation of photoaffinity labeling probes of natural products and pharmaceuticals. **T. Hosoya***, S. Yoshida, Y. Misawa
- 1257.** Divergent synthesis of pseudoenantiomers toward ABC-ring moiety of steroids. **M. Furuta**, K. Hanaya, T. Sugai, M. Shoji*
- 1258.** Structure-activity relationship studies of oligomeric flavan-3-ols: Role of phenolic hydroxyl groups in biological activities. **Y. Hamada**, K. Ito, Y. Ayano, T. Koashi, N. Nakajima, A. Saito
- 1259.** Synthesis of inositol phospholipids from *Ascaris suum* using regioselective phosphorylation. **S. Suehara**, T. Aliba, S. Nakagawa, M. Sato, Y. Maekawa, T. Mura, K. Fukase, S. Inuki, Y. Fujimoto
- 1260.** Synthetic study of the C31-C67 part of amphiindol 3. **Y. Wakamita***, M. Ebine, T. Oishi
- 1261.** Synthetic studies toward strophasterol A. S. Sato, M. Murakami, T. Hirokawa, **S. Kuwahara***
- 1262.** Synthesis of sugar-modified EGCGs by direct C-glycosylation and its application to a chemical biology. **H. Hamagami**, Y. Hatasa, Y. Yamaguchi, S. Fuse, T. Shibata, H. Tachibana, K. Uchida, H. Tanaka
- 1263.** Total synthesis of cyclobakuchiol by using conformation-controlled stereoselective reactions. **H. Kawashima**, Y. Kaneko, M. Sakai, N. OGAWA, Y. Kobayashi*
- 1264.** Synthetic study of the LM ring of maitotoxin. **H. Kishigami**, T. Oishi, M. Ebine, K. Torikai
- 1265.** Synthetic study of tricyclic terpenoids via convergent strategies. **K. Kuwata***, K. Hanaya, T. Sugai, M. Shoji
- 1266.** Synthetic strategy toward unique complex right-side structures of phasins. **M. Morita**, S. Kojima, G. Hirai, M. Sodeoka*
- 1267.** Synthetic studies on iriomoteolide-2a. **K. Sakamoto**, A. Hakamata, H. Fuwa*, M. Sasaki
- 1268.** Synthetic study on cardiolipin containing cyclopropane fatty acids. **S. Ishibashi**, S. Inuki, Y. Fujimoto
- 1269.** Synthetic study of cinerin. **M. Tanigawa**, T. Usuki*
- 1270.** Total synthesis of palau'amine. **K. Takeuchi**, Y. Kaihara, K. Tanino, K. Nam*
- 1271.** Synthetic study of cyclic desmosine for elucidation of the crosslinking structure of elastin. **K. Ogawa**, T. Usuki*
- 1272.** Stereoselective synthesis of resolivins and 12-HHT. **N. OGAWA**, Y. Kobayashi*
- 1273.** Synthetic study of various flavan-3-ol analogs by regioselective modification of 5-position of flavan-3-ols and their structure-activity-related study. **Y. Higashino**, K. Mori, Y. Ayano, T. Hojima, N. Nakajima, A. Saito
- 1274.** Synthesis of funiculosin derivatives as immune activators via TLR4/MD-2. **K. MIZOTE**, A. SAEKI, H. HONDA, N. OKAMOTO, T. KIMURA, Y. NAGAI, K. TAKATSU, Y. Fujimoto*, K. Fukase*
- 1275.** Formal synthesis of madindoline A via enzymatic discrimination of quaternary carbon center. **M. Shoji***, K. Shimizu, M. Tomita, K. Fuhshuku, T. Sugai

- 1276.** Alternative one-pot synthesis of (trifluoromethyl)phenyldiazirines from corresponding tosylxime derivatives for photoaffinity labeling. **L. Wang***, Y. Murai, T. Yoshida, A. Ishida, Y. Sakihama, Y. Hashidoko, M. Hashimoto
- 1277.** Practical synthesis of natural plant-growth regulator 2-azahypoxanthine, its derivatives, and biotin-labeled probes. **K. Ikeuchi**, M. Inai, T. Asakawa, Y. Hamashima, H. Kawagishi*, T. Kan*
- 1278.** Synthetic studies of IUBR-23, -24. **S. Yorita**, H. Yokoyama, M. Miyazawa*
- 1279.** Synthetic studies of Schigglautone A. **H. Yamasawa**, H. Yokoyama, M. Miyazawa*
- 1280.** Synthetic study of the LMNOPOQRS ring system of maitotoxin. **H. Onoue***, K. Torikai, M. Ebine, T. Oishi
- 1281.** Total synthesis of siprofuginin A. **K. Kunichika**, H. Yokoyama, M. Miyazawa*
- 1282.** Studies toward the total synthesis of cynaropinic. **T. Mori**, T. Usuki*
- 1283.** Novel synthesis of zerumbone-pendant derivatives for development of biologically active compounds. **Y. Utaka**, Y. Kawai, T. Kitayama
- 1284.** Synthesis of 1,3a,6a-triazapentalene derivatives and their interesting fluorescence properties. **K. Namba***, A. Osawa, A. Nakayama, A. Mera, A. Otani, K. Tanino
- 1285.** Synthetic study of plusbacin A₃. **A. Katsuyama**, A. Matsuda, S. Ichikawa*
- 1286.** Synthesis and biological activities of the amide derivative of aplog-1, a simplified analog of aplysisatin with antiproliferative and cytotoxic activities. **Y. Hanaki**, R.C. Yanagita, C. Takahashi, T. Sugahara, M. Aida, H. Tokuda, K. Irie*
- 1287.** Synthesis and biological activity of phosphatidylinositol for the elucidation of NKT cell pre-activation mechanism. **S. Nakagawa**, A. Shimoyama, T. Aliba, Y. Fujimoto, F. Kochi*
- 1288.** Synthesis of novel allene-zerumbone derivatives with twelve membered ring. **T. Miyamura**, H. Tatsumi, M. Kameo, T. Kitayama
- 1289.** Synthesis of optically active 3-O-acylated catechin analogs by oxidative cyclization. **N. Shiraiishi**, M. Kumazoe, S. Fuse, H. Tachibana, H. Tanaka*
- 1290.** Fundamental reaction activity of zerumbone with conjugated system in the eleven-membered ring structure for development of biologically active compounds. **A. Nishikawa**, C. Yamamoto, T. Kitayama
- Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1
- The Science and Strategy of Pharmaceutical Process Chemistry: Adapting to Global Regulatory Development Guidance on Process Impurities (#242)**
- Organized by: H. Okuda, T. Watson, G. CHAE
Presiding: T. Watson
- 8:00 Welcome introductions**
- 8:05 – 1291.** Recent efforts in implementation ICH Q11 quality guidance in Japan. **H. Okuda***, K. Takagi
- 8:30 – 1292.** Can ICH Q12 help realise the full benefits for ICH Q11 and enhanced process understanding?. **F. Montgomery***
- 8:55 – 1293.** Early experiences with ICH Q11: successes and opportunities. **J. Lepore**
- 9:20 – 1294.** ICH Q11 Starting material IWG Update - the role of impurities. **T. Watson**
- 9:45 Break**
- 9:55 Q&A**
- 10:10 – 1295.** Use of models for the development and implementation of a small molecule impurity control strategy. **K.D. Seibert***, C. Luciani, S. Coffey, **K.D. Seibert**
- 10:35 – 1296.** QbD implementation and ICH Q11 application – a case study of life-cycle approach to impurity control. **T. Watson**

- 11:00 – 1297.** Development of manufacturing route to elbasvir. **J. Yin***
- 11:25 – 1298.** Strategies of assessment, analysis, and control of genotoxic impurities in drug substance development with case studies. **H. Lee***

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Molecular Self-Assembly and Functional Organic Nanostructures (#263)

Organized by: J. Parquette, M. Lee, J. Badjic, F. Huang
Presiding: J. Badjic

8:00 Introductory Remarks

- 8:10 – 1299.** Electronic delocalization within self-assembled nanostructures derived from pi-conjugated oligopeptides. **J.D. Tovar***

- 8:40 – 1300.** Complex topologies through subcomponent self-assembly. **J.R. Nitschke***

- 9:10 – 1301.** Cooperative supramolecular polymerization of hydrogen-bonded supermacrocycles. **M. Yamauchi***, S. Yagai*

9:40 Coffee Break

- 9:55 – 1302.** Shape-selective synthesis and self-sorting of covalent organic cage compounds. **F. Beuerle***

- 10:25 – 1303.** Surface-supported robust 2D lanthanide-carboxylate coordination networks. **B. Cirera, J. Urgel, Y. Wang, W. Auwarter, H. Otero, J. Gallego, M. Alcamí, S. Klyatskaya, M. Ruben, F. Martin, R. Miranda, J. Barth, D. ECIJA**

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Molecular Probes and Fluorophores for Biological Imaging (#280)

Organized by: C. Fahrni, C. Cairo, C. Yip, Y. Horie
Presiding: Y. Horie

8:00 Opening Remarks

- 8:05 – 1304.** Development of imaging agents to target tumour hypoxia. **D. Sneddon**, R. Niemans, N.G. Lieuwe, R. Biemans, M. Bauwens, I. Pooters, L. Dubois, P. Lambin, P. Pellegrini, N. Lengkeek, C.T. Supuran, S. Poulsen*

- 8:25 – 1305.** Phosphorescent probes for multiphoton microscopy of oxygen. **S. Vinogradov***

- 8:45 – 1306.** HKSOX series of highly selective and sensitive fluorescent probes for multiplatform detection of superoxide in live cells and *in vivo*. **J. Hu, N. Wong, S. Ye, D. Yang***

- 9:05 – 1307.** Long(er) wavelength fluorescent probes. **K. Gee**

- 9:35 – 1308.** Illuminating metals: Fluorescent tools for the study of cellular magnesium. **M. Afzal, J. Gruskos, J. Pitteloud, G. Zhang, D. Buccella***

10:05 Session Break

- 10:20 – 1309.** Fluorescent probes based on sulfur as a reporting element. **N. Finney**

- 10:40 – 1310.** Towards targeted ratiometric sensors of labile metal pools. **C. Shen***, I. Carney, K. Yang, E. New

- 11:00 – 1311.** Spectroscopic probes and sensing analysis (2015). **H. Ma**

- 11:30 – 1312.** Tunable molecular-based nanoparticles as biocompatible and eco-friendly alternative to quantum dots for bioimaging. **M.H. Blanchard-Desce**

Hawaii Convention Center
Halls I, II, III

Frontiers of Chirality in Organic Chemistry (#286)

Organized by: J. Canary, N. Berova, E. Yashima, M. Hyun, T. Shibata, T. Asahi, C. Welch, S. You
Presiding: T. ASAHI, N. Berova,

J. Canary, M. Hyun, T. Shibata, C. Welch, E. Yashima, S. You

Poster Session

10:00 – 12:00

Spontaneous Resolution and Autocatalysis

- 1313.** Spontaneous formation of enantioenriched α -amino nitrile, chiral precursor of Strecker synthesis. **T. Kawasaki***, N. Takamatsu, S. Aiba, Y. Tokunaga

- 1314.** Asymmetric synthesis of nitrogen isotopically chiral diamine and its chiral discrimination by asymmetric autocatalysis. **H. Ozaki**, K. Tada, S. Harada, T. Ayugase, H. Ozawa, T. Kawasaki, A. Matsumoto, K. Soai*

- 1315.** Asymmetric autocatalysis triggered by helical arrangement of chiral crystals of achiral organic compounds. **Y. Kaimori**, T. Ide, S. Fujiwara, M. Uchida, T. Sasagawa, T. Kawasaki, A. Matsumoto, K. Soai*

Chiral Materials and Nanostructures

- 1316.** Control of metal arrays based on heterometallics masquerading in heterochiral aggregations of chiral clothe spins-shaped complexes. **M. Naito***, R. Inoue, S. Kawamorita, N. Komiyama, T. Naota

- 1317.** Synthesis of *N*-hetero-*ortho*-phenylene oligomers containing pyridyl groups. **Y. Tokoro***, N. Ohtsuka, A. Toh, S. Fukuzawa*

- 1318.** Synthesis and acid/base-triggered extension/contraction motion of a double-stranded boron helicate bearing bipyridyl units. **Y. Suzuki**, T. Nakamura, S. Yamamoto, D. Taura, H. Iida, N. Ousaka, E. Yashima*

- 1319.** Helix inversion of β -peptide by hydrogen bonding pattern alteration. **S. Shin**, Y. Kim, I. Guzei, S. Choi*

- 1320.** Synthesis and application of complementary double helices connected with metal-salen complexes. **S. Hioki**, J. Tanabe, D. Taura, E. Yashima

Chiral Analysis, Recognition, and Separation

- 1321.** High throughput analysis of enantio-purity in pharmaceutical research using multiple injections. **K. Zawatzky**, E.L. Regalado, C. Welch

- 1322.** Discrimination of chiral crystals with two-fold screw axis using optical activity. **K. Ishikawa***, Y. Terasawa, M. Tanaka, M. Shiro, H. Koshima, T. ASAHI*

- 1323.** Solvent-induced kinetic and thermodynamic control of remote-controlled planar chirality in peptide-bound metallocycles. **F. Mamiya**, N. Ousaka, E. Yashima*

- 1324.** Solid-liquid and liquid-liquid extractions of native saccharides by alternating pyridine-phenol oligomers linked with acetylene bonds. **Y. Ohishi**, M. Inouye, H. Abe

- 1325.** Dynamic formation of enantiomeric thalidomide dimeric structure: Solid and solution state chiroptical spectroscopy and computational analysis. **T. Hiroki**, Y. Ogino, M. Tanaka, N. Shibata, T. ASAHI*, T. SHIMOZAWA

- 1326.** Synthesis and application of optically pure rotaxanes with their specific chirality for enantioselective complexation with chiral amines. **K. Hirose**, R. Kano, K. Tsuda, H. Furutani, Y. Hinohara, Y. Tobe*

* Principle Author

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- 1327.** Synthesis and conformational analysis of novel helical amide oligomers.
K. Urushibara, H. Masu, I. Azumaya, H. Kagechika, A. Tanatani*
- 1328.** Highly stereoselective recognition of undervatized amino acids by a simple chiral phenyl aldehyde. **Q. Chen**, k. kim
- 1329.** Efficient resolution of 2-fluorophenylglycine by continuous preferential crystallization. **C. Rougeot***, R.M. Kellogg, J. Hein

Asymmetric Synthesis and Catalysis

- 1330.** Study on the stereoselective cyclization of 1-alkenyl β -aminoalkyl sulfides and sulfones. **M.R. Kulak**, A.L. Schwan, S. Soderman, T. Moek
- 1331.** Development of new synthetic reactions leading to organophosphorus compounds having chiral carbon centers. **Y. Maekawa**, T. Murai

- 1332.** Crystal structure analysis of asymmetric autocatalysis of pyrimidyl alkanol. **A. Matsumoto**, T. Abe, A. Hara, T. Tobita, T. Sasagawa, T. Kawasaki, K. Soai*
- 1333.** Synthesis the planar chiral phosphine-olefin ligand base on the transition metal scaffold and application in asymmetric catalysis. **Y. Tseng***, M. Ogasawara, S. Arae, T. Takahashi, K. Kamikawa

- 1334.** Desymmetrization hydrogenation of a meso-cyclic acid anhydride toward biotin synthesis. **M. Yoshimura**, K. Tsuda, H. Nakatsuka, T. Yamamura, S. Tanaka, M. Kitamura
- 1335.** Diastereoselective synthesis of an axially chiral 2,2'-bipyridine -N,N'-dioxide bearing peptide chains. **A. Urushima**, N. Ousaka, E. Yashima*

- 1336.** Asymmetric synthesis of MnNP acid using a chiral auxiliary. **W. Fujiwara**, M. Kato, M. Kusakari, T. Kijima, S. Murakami, S. Matsuba, B. Hatano*
- 1337.** Asymmetric Suzuki-Miyaura cross-coupling of 1-bromo-2-naphthalenes using helically chiral polymer ligand PQX-phos. **Y. Akai**, T. Yamamoto, M. Sugihara*

- 1338.** Enantioselective synthesis of heterocyclic compounds via asymmetric Heck-Matsuda oxyarylation of styrene-like compounds. **N.C. Martins**, A.R. SILVA, C.D. Correia*
- 1339.** Synthesis of optically organosele-nides using chiral auxiliaries. **Y. Taguchi**, Y. Nakazawa, R. Mashiko, B. Hatano, S. Murakami, T. Kijima

- 1340.** Enantioselective Heck-Matsuda arylations: Synthesis of substituted 2,3-dihydrobenzofurans by a new oxyarylation reaction. **A.R. SILVA**, N.C. Martins, C.D. Correia*

- 1341.** Solvent free chiral inversion of thalidomide and hydrolysis product of thalidomide. **M. Nakamura**, K. Otegawa, T. SHIMIZUWA, T. ASAHI*
- 1342.** Enantioselective synthesis of γ -amino acids via sp³ C-H Bond activation using by Ir(I)-catalyst. **M. Michino**, M. Ito, Y. Tahara, T. Shibata*

- 1343.** Synthesis of phosphonate monoesters via hydrolysis of phosphonate esters having a biphenyl group and their application. **K. Kuwabara***, Y. Maekawa, Y. Hirai, T. Murai
- 1344.** Chiral β -aminoalcohol catalysts with bulky substituents possessing strong asymmetric power determined by competitive asymmetric autocatalysis. **Y. Komuro**, Y. Mori, R. Noto, N. Watabe, T. Kawasaki, A. Matsumoto, K. Soai*

- 1345.** Asymmetric synthesis of planar-chiral functionalized paracyclophanes and their application as chiral ligands. **M. Fukai**, H. Madhurima, R. Sekine, S. Oshima, T. Shibata*
- 1346.** Ag(I)-bisamidine catalyzed asymmetric Friedel-Crafts alkylation of indoles with α -substituted- β -nitroacrylates. **T. Nomoto**, M. Yamanaka*

- 1347.** Enantioselective synthesis of aminodane carboxylic acid derivatives by the Rh-catalyzed [2+2+2] cycloaddition. **S. Obinata**, Y. Tahara, T. Shibata*
- 1348.** Catalytic enantioselective synthesis of P-stereogenic phosphine derivatives by molybdenum-catalyzed asymmetric ring-closing metathesis on (π -arene)chromium platform. **M. Ogasawara**, R. Ikehata, Y. Tseng, W. Wu, S. Arae, R. Yasuda, T. Takahashi, K. Kamikawa

- 1349.** Asymmetric synthesis of triptycene via enantioselective alkynylation of 1,5-di-bromoanthracene-9,10-dione. **Y. Kamimura**, T. Shibata*
- 1350.** Asymmetric hydrogenation of quinazolinium salts catalyzed by dinuclear iridium(II) complexes bearing chiral diphosphine ligand. **K. Higashida**, A. Iimuro, Y. Kita, K. Mashima*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Fluorinations and Fluoroalkylations (#310)

- Organized by:* S. Prakash, T. Ritter, K. Mikami, S. Fustero, J. Hu
Presiding: K. Mikami

8:00 Opening Remarks

- 8:05 – 1351.** Studies on fluoroalkylations. **S. Prakash***

- 8:30 – 1352.** New version of Umemoto reagent for practical application: Di- and tetra-fluoro-S-(trifluoromethyl)dibenzo-thiophenium salts. **T. Umemoto***, T. Zhu, B. Zhang, Y. Li

- 8:55 – 1353.** Difluoromethylthiolation: New reagents and reactions. **Q. Shen**

- 9:20 – 1354.** Carbene-induced intra- vs. intermolecular transfer-trifluoromethylation of aryl trifluoromethylthio-compounds under rhodium catalysis. **N. Shibata***

- 9:45 – 1355.** Trifluoromethylation of olefins by photoredox catalysis. **M. Akita***, T. Koike

- 10:10 – 1356.** Transition metal catalyzed fluoralkylation with fluoroalkyl bromides and chlorides. **X. Zhang***

10:35 Break

- 10:45 – 1357.** New approach for catalytic asymmetric synthesis of beflexonate. **J. Ma**

- 11:10 – 1358.** Straightforward access to ¹⁸F-labeled PET probes via Ni/Cu co-catalyzed defluoroborylation of fluorarenes. **T. NIWA***, H. Ochiai, Y. Watanabe, T. Hosoya

- 11:35 – 1359.** Monofluorinated building blocks: New synthetic approaches. **S. Fustero***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Organic Solid-State Chemistry: Structure, Property & Reactivity (#398)

- Organized by:* M. Sakamoto, L. MacGillivray, J. Vital
Presiding: M. Sakamoto, R. Tamura

- 8:00 – 1360.** Hierarchical construction of multistructural porous organic salts (POSs) through different networks of supramolecular clusters. **T. Miyano**, A. YAMAMOTO, I. HISAKI, M. MIYATA, N. TOHNAI*

- 8:20 – 1361.** Design of triple vapochromic organic crystals of quinolone antibiotics. **A. Sakon***, A. Sekine, H. Uekusa

- 8:40 – 1362.** Synthesis of chemically-modified 3-tert-butyl benzotriazinyl radicals and their magneto-structural correlation. **Y. Takahashi**, Y. Miura, N. Yoshioka*

- 9:00 – 1363.** Morphological control of organic semiconductor crystals by surface design and matrix rheology. **S. Okada**, M. Oiki, S. Furukawa, H. Tanaka, K. Harano, E. Nakamura*

- 9:20 – 1364.** Controlled cycloaddition reaction mediated by noncovalent interaction. **Y. Ma**, X. Meng

- 9:40 – 1365.** Crystallisation, melt racemisation, and polymorphic transformation of pyroglutamic acid. **H. Wu***, A.R. West

10:00 break

- 10:10 – 1366.** Thermally responsive crystal of cyclic amphiphilic molecule including monodisperse oligoethylene glycol units. **K. Kinbara***, T. Shima, T. Muraoka, N. Hoshino, T. Akutagawa, Y. Kobayashi

- 10:30 – 1367.** Solution and solid-state reactions of the larger acenes. **J. Anthony**, A. Petty

- 11:00 – 1368.** Synchrotron studies of self-compression in chain inclusion compounds. **M.D. Hollingsworth***, B. Wang, I. Frantsuzov, S. Nichols, P. Rabiller, C. Mariette, L. Guérin, B. Toudic

- 11:30 – 1369.** Chemical complexity phenomena observed in chiral crystalline and liquid-crystalline phases. **R. Tamura**

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

New Organosulfur Chemistry (#436)

- Organized by:* E. Block, E. Juaristi, A. Schwan, X. Jiang, C. Lee
Presiding: E. Block, E. Juaristi

8:00 Introductory Remarks by Eric Block

- 8:05 – 1370.** Synthesis and stereochemistry from sulfenic acid anions. **A.L. Schwan***, S.C. Söderman, M.R. Kulak, E. Remigio

- 8:35 – 1371.** Sulfinic acids, selenenic acids, and hydrosulfides: Potent redox mediators or just neat molecules?. **D. Pratt**

- 9:05 – 1372.** New modes of sulfur reactivity for organic synthesis, biochemistry, and polymer science. **J.M. Chalker***, G.A. Edwards, G.H. Jones, M.P. Crockett, A.M. Evans, M. Tierney

- 9:35 – 1373.** Synthesis, structure, and reactivity of a primary-alkyl-substituted sulfinic acid and its anion. **K. Goto***, M. Ishihara, N. Abe, S. Sase

10:00 Break

- 10:10 – 1374.** Formations of organosulfur compounds in disrupted LFS-suppressed onion and their bioactivities. **T. Kamoi**, M. Aoyagi, M. Kato, S. Imai

- 10:40 – 1375.** Odorless synthesis of bioactive sulfur-containing molecules. **T. Wirth***

- 11:05 – 1376.** Characterization and synthesis of novel ring-substituted thiolenes from extracts of crushed garlic (*Allium sativum*). **B. Dethier***, E. Block

- 11:30 – 1377.** Solvent-dependent self-assembly of S-substituted cysteines. **R.A. Musah***, T. He

Thursday Afternoon

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25)

- Organized by:* T. Kubo, Y. Tobe, M. Haley, G. Bodwell, K. Wong
Presiding: T. Kubo

- 13:00 – 1378.** Supramolecular functionalization of nanocarbons with electroactive π -conjugated non-planar recognition motives. **N. Martin**

- 13:40 – 1379.** Tetraphiafulvalene vinyllogues as versatile building blocks: From small molecular systems to nanomaterials. **Y. Zhao***

- 14:05 – 1380.** Expanded indeno-fused carbocyclic and heterocyclic quinoidal scaffolds: Syntheses, structures, and properties. **M.M. Haley**

- 14:30 – 1381.** Straightforward synthesis of highly twisted porphyrin oligomers. **S. Hiroto**, S. Ito, H. Shinokubo

- 14:45 – 1382.** Cyclopentenyl fused acenes and quinoidal heteroacenes. **C. Chi***

- 15:00 – 1383.** Defining the structure, properties, and reactivity of $[n]cumulenes$. **R.R. Tykwinski**

- 15:40 – 1384.** Construction of chiral structures from anthracene units and acetylene linkers. **S. Toyota***, T. Iwanaga

- 16:05 – 1385.** Open-shell π -conjugated molecular systems for nonlinear optics. **M. NAKANO***, R. Kishi, K. Yoneda, K. Fukuda, B. Champagne

- 16:30 – 1386.** Synthesis of novel acenequinones and investigation of their self-assembly. **K. Maly***, J.A. Paquette, R.E. Yardley, E. Cieplechowicz, M. Halloran

- 16:45 – 1387.** Dithienothiazines as novel heterocyclic donors – phenothiazine congeners enriched in electron density. **T.J. Müller***

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41)

- Organized by:* T. Akasaka, F. Wudl, L. Echegoyen, X. Lu, C. Wang
Presiding: H.C. Dorn, D.M. Guldi

- 13:00 – 1388.** Growing carbon nanotubes from synthetic organic end-caps. **L.T. Scott***

- 13:40 – 1389.** Open-cage fullerenes toward endofullerenes and heterofullerenes. **Y. Murata***

- 14:10 – 1390.** Synthesis of polybenzoquinolines as graphene nanoribbon precursors. **Y. Park**, D.J. Dibble, A. Mazaheri-pour, M.J. Umerani, A.A. Gorodetsky

- 14:25 – 1391.** One-shot K-region selective annulative π -extention of polycyclic aromatic hydrocarbons for nanographene synthesis. **H. Ito**, K. Ozaki, M. Shibata, K. Kawasumi, K. Itami*

- 14:40 – 1392.** Organic functionalization of lithium-ion-containing fullerenes. **Y. Matsuo***

- 15:00 – 1393.** Decorating nanocarbons with optoelectronic systems. **A. Astre-Santos***

- 15:20 – 1394.** Electron mobility of zero, 1- and 2D nanocarbons in their bulk states/interfaces. **S. Seki**

- 15:50 – 1395.** Recent structural results reveal shape-compatible cocrystallization agents for tubular-shaped fullerenes. **M.M. Olmstead***, A.L. Balch, K. Ghiasi

- 16:20 – 1396.** Effect of covalent bond formation on the electronic structure, magnetism, and properties of graphene and carbon nanotubes. **R.C. Haddon**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Natural Product-based Drug Discovery (#66)

- Organized by:* B. Baker, R. Kerr, Y. Qin, D. Uemura, B. Littlefield
Presiding: H. OSADA, J. Qi

- 13:00 – 1397.** Biosynthesis study aiming at creation of an anti-osteoclast drug. **H. OSADA***, T. Nogawa, S. Takahashi

- 13:40 – 1398.** Design and synthesis of novel ligands of opioid receptors. **H. Nagase***

- 14:10 – 1399.** Discovery of natural products with activities against the subtypes of triple negative breast cancer. **S.L. Mooberry***

- 14:40 – 1400.** Small molecule derived from natural products for treatment of age-related diseases. **J. Qi**, R. Tang, Y. Luo, K. Sun, L. Xiang

- 15:10 – 1401.** Biological activity of biselyngbyasides, macrolides from marine cyanobacteria. **K. Suenaga**

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TECHNICAL PROGRAM

15:30 – 1402. Drug discovery targeting the ubiquitin-proteasome system from marine organisms. **S. Tsukamoto***

15:50 – 1403. Development of natural product-like library by using diversity-enhanced extracts. **H. Kikuchi***, Y. Oshima

16:00 – 1404. Bioactive and novel metabolites from marine and terrestrial Malaysian fungi. **M.R. Prinsep***, G. Tait, C. Linderboom, F. Lim, S. Lim, K. Ramasamy, A. Cole

16:10 – 1405. Glycolipopptide possessing a branched lipid unit as a TLR2 ligand. H. Koizuma, H. Sugiyama, H. Kiyohara, M. Sunagawa, **H. Tanaka**

16:20 – 1406. Comparison of vanadium dependent bromoperoxidases from three species of the red algal genus *Laurencia*. K. Kaneko, K. Washio, D. Kobayashi, T. Ishikawa, T. Umezawa, F. Matsuda, K. Nishikawa, Y. Morimoto, M. MORIKAWA, **T. Okino***

16:30 – 1407. New cytotoxins from sponges of deeper coral reefs and a marine micro-organism. **J. Tanaka**, P. Ahmadi, T. Wauke, A. Agena

16:40 – 1408. Anti-aging substance from nature products and their mechanism of action. **L. Xiang***, K. Sun*, Y. Weng*, Y. Lin, Y. Sun*, J. Qi*

16:50 – 1409. General, practical, and diversifiable synthetic route to new macrolide antibiotics. **Z. Zhang**, I. Seiple, P. Wright, A. Langlois, K. Yabu, M. Condakes, D. Hog, P. Jakubec

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Molecular Containers (#99)

Organized by: S. Mitsuhiro, L. Isaacs, H. Yang
Presiding: H. Ube, Z.R. Wang

13:00 – 1410. Learning what knot to do. **D. Leigh***

13:30 – 1411. Functional materials from self-assembling bis-urea macrocycles. S.R. Salpage, A.A. Korous, **L.S. Shimizu**

13:55 – 1412. Pillar[n]arene-based supramolecular assemblies for gas storage and porous carbon fibers. **T. Ogoshi***, K. Yoshikoshi, R. Sueto, T. Yamagishi

14:20 – 1413. Functionalized self-assembled cages: Stereocontrol and reactivity. **R. Hooley**

14:45 coffee break

14:55 – 1414. From heterocalixaromatics to coronal[n]arenes. **M. Wang***

15:25 – 1415. Functional container molecules through subcomponent self-assembly. **J.R. Nitschke**

15:55 – 1416. Polyaromatic micelles with wide-ranging host capability in water. **M. Yoshizawa***

16:20 – 1417. Mutual induced fit in artificial molecular systems: Creation of host–host structures. **T. Sawada**, H. Hisada, S. Wang, M. Fujita*

16:40 – 1418. Rotaxane dendrimers with mechanically interlocked moieties on branches. **H. Yang**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100)

Organized by: D. Hall, B. Wang, P. Duggan, M. Sugino

Presiding: M. Sugino

13:00 – 1419. Catalysis based on reversible covalent interactions of organoboron compounds. **M.S. Taylor***

13:30 – 1420. Boron compounds for determining the enantiomeric excess of chiral analytes and as sensors for detecting fluoride, hydroxy radicals, and peroxy nitrite in water. **S.D. Bull**

13:50 – 1421. Benzoxaboroles for membrane separation. **E.V. Lampard***, T.D. James, S.D. Bull, D. Patterson

14:10 – 1422. Developing the phosphinoboration reaction. S.J. Geier, C.M. Vogels, S. Doherty, **S. Westcott***

14:40 – 1423. Hydroxymethylboronic acid and its anhydride-ester dimer. **D.S. Matteson***

15:00 Break

15:10 – 1424. Basic science of azaborines and the progress toward their applications in medicinal chemistry. **S. Liu***

15:40 – 1425. Amino-boro-naphthalenes: From satisfaction to frustration. **E. GRAS***, D.C. Pla Queral, B. Mestre

16:00 – 1426. Development of a novel class of hybrid materials involving boronates and benzoxaboroles. **D. Laurencin***, S. Sene, M. Pizzocaro, S. Bégu, D. Berthomieu, C. Gervais

16:20 – 1427. Chemistry of boron-doped nanographenes. **S. Yamaguchi***

Hilton Hawaiian Village
Rainbow Tower, Rainbow 1

Electrochemical Reactions and Mechanisms in Organic Chemistry (#104)

Organized by: K. Chiba, S. Suga, K. Moeller, C. Frontana
Presiding: C.E. Frontana, D. Little, S. Suga

13:00 – 1428. Competition studies, cyclic voltammetry, and the use of mechanistic insights to guide the design of new radical cation reactions. R. Perkins, L. Gonzalez, M. Graaf, R. Feng, **K.D. Moeller**

13:15 – 1429. Recent advances in the construction and use of functionalized micro-electrode arrays. M. Graaf, S. Uppal, D. Rensing, B. Nguyen, **K.D. Moeller***

13:30 – 1430. Biradical chemistry with electrode: Biradical formation from peroxy radical cation and its reactions. **R. Akaba***

13:45 – 1431. Bipolar electrochemistry for fabricating gradient polymer bushes. **S. Inagi***, N. Shida, Y. Koizumi, H. Nishiyama, I. Tomita

14:00 – 1432. Molecular design and synthesis of D-π-A dye sensitizers with pyridyl group for high-performance dye-sensitized solar cells. **Y. Oyama***

14:15 Break

14:30 – 1433. Reactions of electrochemically generated β-haloalkylosulfonium ions. **R. Hayashi**, Y. Ashikari, T. Nokami, A. Shimizu, J. Yoshida*

14:45 – 1434. Reductive acylation and trifluoracetylation of aromatic conjugated yrones by electron transfer from magnesium. **T. ZHANG***, Y. NISHIYAMA, H. MAEKAWA

15:00 – 1435. Transformation of regioregular organotitanium polymers into π-conjugated polymers containing Group 16 elements. **N. Hiroki**, S. Inagi, I. Tomita

15:15 – 1436. Synthesis of fluorinated tetrahydropyrans via Prins cyclization of aldehydes and homocyclic alcohols using electrochemical oxidation.

K. Matsumoto*, K. Yamaguchi, K. Miyasaka, F. Haga, T. Nokami, K. Nishiwaki, S. Kashimura

15:30 Break

15:45 – 1437. Advances in anodic C,C-cross-coupling reactions of phenols and arenes. **A. Wiebe***, S.R. Waldvogel, R. Franke, K.M. Dyballa

16:00 – 1438. Stability and reactivity of thienium ions generated by electrochemical oxidation. **S. Horiechi**, R. Hayashi, A. Shimizu, J. Yoshida*

16:15 – 1439. Direct observation and reactivity of thionium ions generated by using the indirect cation pool method.

A. Shimizu, K. Takeda, K. Saito, S. Kim, T. Nokami, J. Yoshida*

16:30 – 1440. Catalytic activity of electrochemically generated organo-dications. **S. Suga***, I. Fujiwara, Y. Kurihara, Y. Onishi, K. Mitsudo

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Recent Trends in Organocatalysis (#122)

Organized by: M. Terada, M. Shi, J. Antilla, K. Maruoka
Presiding: K. Maruoka, M. Shi, M.P. Sibi, W. Wang

13:00 – 1441. Recent advances in organocatalytic bromination reactions. **Y. Yeung***

13:30 – 1442. Zwitterion directed regio- and enantioselective cyclizations. **M. Shi***

14:00 – 1443. Enantioselective synthesis of chiral biaryls by means of chiral phosphoric acid. **T. Akiyama**

14:30 – 1444. Cooperativity in catalysis: A novel method for enantioselective transformations with complex substrates. **M.P. Sibi***, H. Subramanian, R. Moorthy

15:00 – 1445. Hetero-Michael addition to α,β-unsaturated carboxylic acids. **Y. Takemoto**

15:30 – 1446. Anilines-mediated organocatalytic reactions. C. Yu*, H. Huang*, X. Li, **W. Wang***

16:00 – 1447. Chiral nucleophilic carbenes for use in organic synthesis: From acyl anion chemistry to internal redox catalysis and beyond. **T. Rovis***

16:30 – 1448. Design of new organoradical catalysts for selective C–H activation and asymmetric cyclization. **K. Maruoka***

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

The Science and Strategy of Pharmaceutical Process Chemistry: Adapting to Global Regulatory Development Guidance on Process Impurities (#242)

Organized by: H. Okuda, T. Watson, G. CHAE
Presiding: F. Montgomery

13:00 Introduction

13:05 – 1449. Challenges in the development of naloxegol: Controlling quality through a 5 stage telescope. **G. Ford***

13:30 – 1450. Use of contextually accurate impurities in spike-challenge studies with proteomics analytics to inform process control strategy, validation, and design space. **R.A. Hart***

13:55 – 1451. Process understanding and its role in a comprehensive control strategy: A case study. **J. Lepore***

14:20 – 1452. Use of ICH Q11 principles in selection of starting materials. **F. Montgomery***

14:45 Questions and Answers

14:55 Break for Coffee

15:10 – 1453. Real time monitoring of quality attributes in mammalian bioprocesses. **C. Wu***

15:35 – 1454. Characterization and development of particles using Raman and FBRM technology in manufacturing. **C. Orihuela**

16:00 – 1455. Fluorometric and colorimetric methods for quantifying palladium in pharmaceuticals. **K. Koide***, M. Tracey, X. Bu, J. Jo, M. Williams, C. Welch*

16:25 – 1456. Novel method of detecting very low levels of polymorphs and other solid forms using high resolution X-ray powder diffraction (XRPD) with a synchrotron light source which allows the detection and quantification of contaminants (of different solid state forms). **L. Cotarca***

16:50 Questions and Answer Session

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Molecular Self-Assembly and Functional Organic Nanostructures (#263)

Organized by: J. Parquette, M. Lee, J. Badjic, F. Huang
Presiding: J. Parquette

13:00 Introductory Remarks

13:10 – 1457. Supramolecular design of self-delivering drugs and imaging agents. **H. Cui***

13:40 – 1458. Stimuli-responsive metal-organic frameworks. **S. Saha***

14:10 – 1459. Self-assembly of highly-crystalline and stable nanosheets from peptide-mimetics. **C. Chen***, Y. Chen, H. Jin, f. Jiao, M. Daily

14:40 – 1460. Aromatic gain as a driving force for supramolecular polymerization. **R. Kielyka***

15:10 Coffee Break

15:25 – 1461. Polar self-assembled molecular materials. **D. Gonzalez Rodriguez***, J. Guilleme, T. Torres, M. Mayoral

15:55 – 1462. Self-assembly of tripodol triptycenes into a highly ordered “2D + 1D” structure. **N. Seiki**, Y. Shoji, T. Kajitani, F. Ishiwari, T. Fukushima*

16:25 – 1463. Fabrication of asymmetric constructions via predesigned chiral mediums . Y. Zhang, **J. LIU***

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Molecular Probes and Fluorophores for Biological Imaging (#280)

Organized by: C. Fahrni, C. Cairo, C. Yip, Y. Hori
Presiding: C. Fahrni

13:00 Opening Remarks

13:05 – 1464. Hip to be square: Building better fluorophores with azetidine. **L. Davis***

13:35 – 1465. Development of luminescent transition metal complexes as bioimaging and cellular reagents. **K. Lo***

14:05 – 1466. Development of protein-labeling probes with fluorogenic switches for imaging cellular events. **Y. Hori***

14:35 – 1467. Fluorescent monitoring of siRNA by modification with dye pairs in cell. **Y. Kamiya**, A. Ito, H. Kashida, H. Asanuma

14:55 Session Break

15:10 – 1468. Tailoring chromophore dark states for improved fluorescence microscopy. **R. Dickson**

15:40 – 1469. Super-resolution fluorescence imaging by dSTORM. **M. Sauer***

16:10 – 1470. Super-resolution imaging in cells using single molecules places new requirements on fluorophore labels. **W. Moerner***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Fluorinations and Fluoroalkylations (#310)

Organized by: S. Prakash, T. Ritter, K. Mikami, S. Fustero, J. Hu
Presiding: J. Hu

13:00 – 1471. New frontier in fluorine chemistry. **K. Mikami***

13:25 – 1472. Difunctionalization-type trifluoromethylation of alkenes. **M. Sodeoka***

13:50 – 1473. Ingenious ecarboxylative route to organofluorine compounds. **H. Amii**

* Principle Author

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14:15 – 1474. Copper catalyzed methane and primary C–H bonds functionalization: The role of fluorine in the $Tp^{(CF_3)_2Br}$ ligand. A. Olmos, B. Noverges, R. Gava, D. Bellezza, T. Varea, A. Caballero, P. Perez*, G. Asensio*

14:40 – 1475. Transformation of tetrafluoroethylene via transition metal intermediates. S. Ogoishi*

15:05 Break

15:15 – 1476. Stereochemically defined C–F fluorine as a new probe of protein-ligand binding sites and enzyme mechanisms. C.E. McKenna*

15:40 – 1477. $SF_5(CF_2)_n$ -containing reagents for synthesis of new fluorinated building blocks. G. Haufe*, P. Dudzinski, A.V. Matsnev, J.S. Thrasher

16:05 – 1478. Preparation and reactions of trifluoromethyl- λ^3 -tetrafluorosulfanes. J.T. Welch*, L. Zhong,

C.N. von Hahnmann, K.A. Gordon

16:30 – 1479. New developments to introduce the difluoromethylene phosphonate fragment. G. Roeschenthaler*

16:55 Closing Remarks

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Organic Solid-State Chemistry: Structure, Property & Reactivity (#398)

Organized by: M. Sakamoto, L. MacGillivray, J. Vittal
Presiding: M.D. Hollingsworth, S. Kohmoto

13:00 break

13:10 – 1480. Thiosemicarbazones: The potential candidates for crystal engineering applications. M.M. Naseer*

13:30 – 1481. Anion networks (evn. chiral) based on halogen bonding interactions. M. Fournier, J. Lieffrig, O. Jeannin

13:50 – 1482. Reaction kinetics in photomechanical molecular crystals. C. Bardeen*, M. Hanson, R. Al-Kaysi, f. tong, l. zhu, t. kim

14:20 – 1483. Size-dependent mechanical properties of organic cocrystals. A.V. Tivanski

14:50 break

15:00 – 1484. Hierarchical construction of diamond porous organic salts (d-POS) and their versatile functions. N. TOHNAI*, A. YAMAMOTO, I. HISAKI, M. MIYATA

15:30 – 1485. Color-tunable solid-state emission of multicomponent crystals by cooperative electron donor-acceptor complexation. T. Ono*, Y. Hisaeda

16:00 – 1486. Gases transform organic solids from one crystal form to another. J.L. Atwood*, S.J. Dalgarno, P. Thallapally

16:30 – 1487. Solid state photo polymerization via [2+2] cyclorxn reaction. J.J. VITTALE, I. Park, S. Lee

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

New Organosulfur Chemistry (#436)

Organized by: E. Block, E. Juaristi, A. Schwan, X. Jiang, C. Lee
Presiding: C. Lee, A.L. Schwan

13:00 – 1488. Electrogeneration, characterization, and reactions of cationic organosulfur intermediates in organic synthesis. J. Yoshida*

13:30 – 1489. Electron transfer through alternating S–π chains: A biological molecular wire?. R. Glass*, N. Monney, T. Yamamoto, T. Bally*

14:00 – 1490. Influence of heavier group 14 elements on [FeFe] diithiolate hydrogenase model complexes. W. Weigand*

14:30 – 1491. Rhodium-catalyzed synthesis of organosulfur compounds. M. Arisawa*

15:00 Break

15:10 – 1492. Changes in properties of sulfur containing microbial chelator by nano-confinement. P. Chatterjee*, I. Sanchez-Lombardo, D.C. Crans*

15:30 – 1493. Topochemical polymerization of S_2N_2 to (SN)_x and the quest towards selenium-containing analogs of chalcogen nitride polymer. O.J. Pakkanen, T.T. Takalo, J.M. Rautiainen, R.S. Laitinen*

15:50 – 1494. Polyimido sulfur scorpionates in metal coordination. D. Stalke*

16:10 – 1495. Versatility of thiocarbonyl compounds in the synthesis of chiral sulfur heterocycles. M. Gulea*

16:35 – 1496. Thioumides for new reactions and new fluorescent molecules. T. Murai*

Thursday Evening

Hawaii Convention Center
Halls I, II, III

Reactive Intermediates and Unusual Molecules (#7)

Organized by: R. Sheridan, M. Abe, W. Leigh

Poster Session

19:00 – 21:00

1497. Synthetic challenges and characterization during the realization of polyyne metallocorporell complexes consisting of axial binding. V. Walter, N. Grzegorzek, N. Jux, F. Hampel, R.R. Tykwiński*

1498. Photochemical generation of 4,4-dialkoxy-1,2-diazacyclopentane-3,5-diyls and their reactivity. S. Yoshidomi*, M. Abe

1499. Reaction of alkoxy radicals with pyridine bases yields pyridinyl radicals that chain amplify photochemical fragmentation of *N* alkoxy pyridinium salts. D. Shukla*, S. Farid, J.P. Dinoccenzo

1500. Excited state C–C bond cleavage-luminescence phenomenon of diarylmethylenecyclopropanes. Y. Matsui, T. Kido, E. Ohta, H. Ikeda*

1501. Stannyl lithium: Facile preparation leading to further synthetic applications. D. Wang, C. Wang, M. Uchiyama

1502. Hypervalent sulfur compound in protein reaction. T. Nakamura*, M. Abe, T. Inoue

1503. Substituent effect on the ground state spin-multiplicity and molecular structure in cyclobutan-1,3-diyldene dicarbenes: Formation of the bicyclo[1.1.0]but-1(3)-ene structure. Y. Fujita*, M. Abe, T. Suzuki, Y. Shiota, K. Yoshizawa

1504. Stretch effect induced by planar skeleton in a macrocyclic system on the chemistry of diradicals. K. Onishi*, M. Abe, S. Hatano

1505. Development of cross-coupling reaction between enol derivatives and silyl ketene acetals catalyzed by gallium trihalides. Y. Nishimoto*, Y. Kita, M. Yasuda, A. Baba

1506. Hypervalent diaryl- λ^3 -bromane-mediated iodine/triflate exchange of iodoalkanes: Direct arylation of iodoalkanes with diaryl(triflate)- λ^3 -bromane. R. Kawasumi*, K. Miyamoto, Y. Masumoto, M. Uchiyama

1507. 1,1-Dichloro-2-nitroethene: A reactive intermediate for heterocycle construction and nitroacetylation of amines. X. Shao

1508. Silicon analog of the smallest bridgehead alkene. N. Akasaka*, S. Ishida, T. Iwamoto

1509. Generation of arynes and cycloalkynes via a sulfoxide–magnesium exchange reaction of readily synthesized precursors. S. Yoshida, K. Uchida, F. Karaki, T. Hosoya*

1510. Mechanistic study on direct aryl transfer of diaryliodane(III) with aryl iodide. Y. Masumoto*, T. Iuchi, M. Ochiai, K. Miyamoto, M. Uchiyama

1511. Fate of NHCl-stabilized dicarbon. D.C. Georgiou, J.L. Dutton*

1512. Quinoidal heteroacenes with bipolar character. X. Shi, C. Chi*

1513. Synthesis of organobismuth compounds by carbobismuthination of alkynes and alkenes using bismuth trihalides and ketene silyl acetals. Y. Nishimoto, M. Takeuchi, M. Yasuda, A. Baba*

1514. Development of a fast spin-state switching system triggered by photolysis. C. Shimokawa*, S. Hatano, M. Abe

1515. Transition metal-free regioselective α -C–H amination of ethers at ambient temperature: Radical-induced amination using (diacetoxyiodobenzene)sulfonamide. J. Yamashita*, K. Miyamoto, M. Uchiyama

1516. Iodoarene-catalyzed Hofmann rearrangement of primary amides. Y. Sakai*, K. Miyamoto, S. Goda, J. Yamashita, M. Ochiai, M. Uchiyama

1517. Triboluminescence and functional properties of trifluoromethylphenyl substituted phthalimide derivatives. J. Nishida*

1518. Structure and chemistry of multiply-charged fluoranyl cations. A. Sumita, Y. Otani, T. Ohwada, K. Giuffre, K. Boblak, M. Gascon, D.A. Klumpp

1519. Efficient generation method and remarkable reactivities of 3-triflyoxyaryne. K. Uchida, S. Yoshida, K. Igawa, K. Tomooka, T. Hosoya*

1520. Unexpected formation of a phenonium ion-containing salt in SET reaction of a cage compound. Y. Kuramoto*, Y. Matsui, E. Ohta, H. Ikeda*

1521. Reaction mechanism and solvent effect in diastereoselective hydride reduction of α -substituted propiophenones. D. Kaneno, H. Saigo

1522. Regio- and stereoselective carboindation of ynl ethers using indium tribromide and silyl enolates. K. Kang*, Y. Nishimoto, M. Yasuda*

1523. Chemistry of tetra-, penta-, and hexacationic systems. M. Gascon*, R. Nareda, D.A. Klumpp*

1524. Palladium catalyzed cross coupling reactions with verdazyl free radicals. D.J. Brook, T. Le, T. Hom, M. Tran, J. Chou

1525. Mechanism of 4-substituted pyrazolones from morta–baylis–hillman adducts elucidated by ESI-MS monitoring. B.V. Ferreira, R.C. Barcelos, L.A. Zeoly, M.T. Rodrigues Jr, M.N. Eberlin*, F. Coelho*

1526. Barrier to phenyl rotation in fluorinated cis-azobenzene. W. Brittain*, P. Rinaldi, A. Rogers, S. Rastogi

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41)

Organized by: T. Akasaka, F. Wudl, L. Echegoyen, X. Lu, C. Wang

Presiding: L. Echegoyen

19:00 – 1527. Phthalocyanine- and subphthalocyanine-containing carbon nanostructures. T. Torres*, O. Trukhina, M. Ragoussi, M. Medel, G. Lavarda, M. Revuelta, L. Mateo, D. Medina, B. Kuhn, G. de la Torre, G. Bottari

19:30 – 1528. Fabrication and photoproperty of coaxial nanowires having carbon nanotube core. Y. Takaguchi*

19:50 – 1529. Methane as a reactive gas in the synthesis of endohedral metallofullerenes. K. Junghans, A. Popov*

20:10 – 1530. Synthesis and properties of substituted sumananes. H. Sakurai

20:30 – 1531. Tumor-targeting diagnosis/therapy multifunctional gadofullerene materials based on $Gd@C_{82}$. C. Wang*, C. Shu

Hawaii Convention Center
Halls I, II, III

Electrochemical Reactions and Mechanisms in Organic Chemistry (#104)

Organized by: K. Chiba, S. Suga, K. Moeller, C. Frontana

Poster Session

19:00 – 21:00

1532. Electrochemical hydrogenation of toluene and o-xylene using a PEM reactor. K. Takano*, T. Kashiwagi, K. Nakabayashi, S. Mitsushima, M. Atobe

1533. Synthesis of polyaniline-poly(methyl methacrylate) core-shell nanocomposites and their application to novel electro-responsive structural colored materials. T. Kuno, K. Nakabayashi, M. Atobe

1534. Stereoselective synthesis of piperidine derivatives using the indirect cation pool method. D. Yamamoto*, T. Akagi, M. Haisa, K. Mitsudo, S. Suga*

1535. Iridium-catalyzed dehydrogenative cyclization leading to dithienosilole derivatives and their electrochemical properties. R. Isobuchi*, K. Mitsudo, S. Suga*

1536. Dye-sensitized solar cells based on ellipsoid titanium dioxide nanoparticles. A. Seki, Y. Shimoyama, T. Kikuchi, K. Tomita, Y. Kunugi

1537. New water-soluble NIR luciferin analog for in vivo imaging. S. Higashi*, R. Saito, M. Kiyama, S. Iwano, N. Kitada, T. Hirano, H. Niwa, S. Maki

1538. Unique cyclization-aromatization reactions of bis(dithienylethenyl)thiophene derivatives promoted by photoinduced electron transfer. A. Yamamoto*, T. Ogaki, E. Ohta, Y. Matsui, K. Mizuno, H. Ikeda*

1539. Ionic liquid tags for electrochemical glycosylation. N. Sasaki, Y. Isoda, Y. Fukaya, T. Nakami*, T. Itoh*

1540. Anodic approach toward intermolecular carbon–carbon bond formations in lithium perchlorate/nitromethane electrolyte solution. Y. Okada, K. Chiba*

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Recent Trends in Organocatalysis (#122)

Organized by: M. Terada, M. Shi,

J. Antilla, K. Maruoka

Presiding: T. Akiyama, K. Nagasawa

19:00 – 1541. Transition-state stabilization through multiple attractive non-covalent interactions in organocatalysis: A computational study. M. Yamamoto*

19:20 – 1542. Activation of the leaving group in the chiral phosphoric acid-catalyzed intramolecular asymmetric S_N2' reaction. K. Yamada*

19:40 – 1543. Enantioselective phase transfer catalysis using pentaniliums. C. Tan

20:00 – 1544. Boron tribromide-assisted chiral phosphoric acid catalysts for highly enantioselective Diels–Alder reaction of 1,2-dihydropyridines. M. Hatano, Y. Goto, K. Ishihara*

20:20 – 1545. Asymmetric halofunctionalization of olefins with novel bifunctional organocatalysts. Y. Hamashima

* Principle Author

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Hawaii Convention Center
Halls I, II, III

The Science and Strategy of Pharmaceutical Process Chemistry: Adapting to Global Regulatory Development Guidance on Process Impurities (#242)

Organized by: H. Okuda, T. Watson, G. CHAE

Poster Session
19:00 – 21:00

1546. Verifying dehydration of hydrolysis compound of thalidomide. **K. Otogawa**, Y. Ogino, K. Ishikawa, T. SHIMOZAWA, M. Tanaka, H. Koshiba, M. Shiro, T. ASAHI*

Hawaii Convention Center
Halls I, II, III

Molecular Self-Assembly and Functional Organic Nanostructures (#263)

Organized by: J. Parquette, M. Lee, J. Badjic, F. Huang

Poster Session
19:00 – 21:00

1547. Accumulation control of polyaromatic molecules through incorporation into single-walled bilayer membrane nanotubes. **Y. Okazaki**, R. Sakaguchi, M. Takafuji, H. Ihara*

1548. Towards electronic communication in redox-active nanotubes. **J.J. Henkelis**, J. Stoddart*

1549. Preparation of water-soluble porphyrin derivatives carrying oligoethylene glycol chains and self-assembly behaviors in water. **T. Tateyama**, S. Karasawa*, N. Koga*

1550. Entropically dominated rotaxanes from rigid pyrene macrocycles. **A. Prokofjevs**, J. Stoddart

1551. Synthesis of rigid triangular molecular prisms. **I. Popovs**, J. Stoddart*

1552. Novel approach to prepare long-range crystalline ultrathin films for organic electronics. **R.H. Fink***, N. Zeilmann, X. Du, S. Pechmann

1553. Conformational dynamics and self-assembly of folded discotic mesogens. **V.E. Williams***

1554. Catalysis of the inversion of bowl-shaped aromatics within cationic receptors. **E.J. Dale***, N.A. Vermeulen, I.C. Gibbs-Hall, K.K. Baldridge, J. Siegel, J. Stoddart

1555. Ruthenium complex-bound amino acid-catalyzed oxidation of methoxyarenes. **R. Yoshida***, K. Isozaki, Y. Yokoi, H.R. Takaya, M. Nakamura

1556. Chemical conversions of hexadecyl self-assembled monolayers based on vacuum ultraviolet irradiations in an atmospheric condition. **A.I. Soliman***, T. Utsunomiya, T. Ichii, H. Sugimura

1557. Concerted pericyclic thermally controlled reactions as a route to design surface-confined functional polymers. **B. Cirera**, G. Nelson, J. Björk, F. Peña, A. Martín-Jiménez, J. Rodríguez-Fernández, A. Pizarro, R. Otero, J. Galan-Mascaros, D. ECIJÁ

1558. Formation of a 2D C₆₀ sheet directed by a tripodal triptycene scaffold. **F. Leung**, F. Ishiwari, T. Kajitani, Y. Shoji, A. Saeki, S. Seki, T. Fukushima*

1559. Effect of the substituted groups at the terminal position of the fluorine-based organic gelators. **Y. Kaneshige**, Y. MORITA, H. OKAMOTO

1560. Characterization of phospholipid vesicles prepared in CO₂/H₂O system at high pressure. K. Suga, S. Taguchi, K. Hayashi, Y. Okamoto, H. Nakamura, H. Umakoshi*

1561. Optical properties of supramolecular gel functionalized by rhenium complexes. **A. Kamo**, Y. Kuwahara*, M. Takafuji, H. Ihara*

1562. Synthesis and phase behavior of nucleobase-containing block copolymers. **E. Kim**, J. Kim*

1563. Preparation of urenylary derivatives carrying one and two amphiphilic chains and their self-assembly behaviors in water. **Y. Okamoto**, E. Ohashi, S. Karasawa*, N. Koga*

1564. Synthesis and gelation ability of 4-perfluoroalkylbutoxybenzene derivatives. **B. Cao**, Y. MATSUE, Y. MORITA, H. OKAMOTO

1565. Mannitol-based amphiphiles (MNAs) for membrane protein structural study. **H. Hussain**, P. Chae

1566. Novel and accessible xylene-linked maltose amphiphiles (XMAS) for membrane protein manipulation. **K. Cho**, P. Chae

1567. Radical templated catenation. **I.C. Gibbs-Hall**, J. Stoddart*

1568. Solid-state polymerization and physical properties of butadiene derivatives with gelation ability. **K. Kikuchi**, Y. Tatewaki, S. Okada*

1569. Preparation of artificial monosaccharide with benzyl group modified cyclo-dextrins. **S. Iida**, S. Fujiwara, K. Takahashi

1570. Cascading effect of copper in click reaction between radical species. **Y. Wang**, J. Sun, Z. Liu, J. Stoddart*

1571. Interaction between hesperidine and various cycloligoglucoside in aqueous solution. **A. Hosaka**, K. Ozawa, K. Takahashi

1572. Water-soluble hydrogen-bonded supramolecular assemblies of perylene bisimide. **I. Fukuda**, S. Yagai

1573. Influence of alkali metal ions on aggregation behavior of crown-ether surfactants. **M. Suzuki**

1574. Preparation of amylose-polypeptide inclusion complexes by vine-twining polymerization. **R. Gotanda**, K. Yamamoto, J. Kadokawa*

1575. Design and synthesis of an effective-volume controllable molecule by redox reaction to trigger the macroscopic motion of self-assembly. **Y. Kurokome**, Y. Kageyama, S. Takeda*

1576. Photoresponsive supramolecular assemblies of azobenzene-linked perylene bisimide. **T. Suzuki**, S. Yagai

1577. Self-assembly of noncovalent supermacrocycles of oligothiophenes in aqueous system. **H. Uchi**, S. Yagai

1578. Naphthalene diimide-based electronically active molecular aggregate. **S. Egami**, N. Fujita*

1579. Synthesis of multiporphyrin assembly using cyclodextrin-bound tetraphenylporphyrin conjugate. **T. Yamashiro**, K. SASAKI

1580. Control over pathway complexity in supramolecular polymerization through modulating the energy landscape by molecular design. **T. Fukui**, S. Ogi, K. Sugiyasu*, M. Takeuchi*

1581. Novel strategy of structure determination of the complicated molecular packing structure of foldecture with PXRD. **J. Gong***, J. Eom, R.W. Driver, H. Lee*

1582. Photothermal assembling of porphyrin dimers. **Y. Yamamoto**, Y. Nishimura, T. Tanaka, H. Yorimitsu, A. Osuka, S. Tokonami, T. Iida*

1583. Abundant mesostructures in self-assembled LC minidendrons. **Y. Liu***, G. Ungar, V. Percec

1584. Reverse amphiphiles having a lipophilic ion pair as the hydrophobic part. **T. Yamada**, K. Kokado*, K. Sada*

1585. Barbiturated naphthalenes with flexible oligo(ethyleneglycol) side chains. **K. Aratsu**, S. Yagai

1586. Comparative analysis of correlation between the secondary structures and self-association behavior of α -peptides. **L. Baek**, R.W. Driver, S. Kwon, H. Lee*

1587. Aggregation behavior of amphiphilic calix[4]resorcinarene. **S. Bingo**, T. Ogoshi, T. Yamagishi

1588. Self-assembly and structural transformation of amphiphilic perylene bisimide dyads. **M. Ogasawara**, X. Lin, S. Yagai

1589. Water-induced helical aggregation of alkylene-tethered perylene bisimide dyads with hydrophilic swallow-tails. **X. Lin**, S. Yagai

1590. Self-assembly of barbiturated oligophenylene: Spontaneous transition of nanostructures from coil to ribbon. **K. Wakita***, S. Yaga*

1591. Supramolecular self-assembled smart dendritic organogels: Rational design and their multiple stimuli-responsive properties. **Y. Feng**, Z. Liu, Q. Fan

1592. Synthesis of porphyrin dimer toward construction of multi porphyrin assembly with molecular recognition sites. **K. Takimoto**, K. SASAKI

1593. Fabrication and self-assembly of resonance core assisted gelators derived from cyclohexanone. **Y. Zhang**, J. LIU

Hawaii Convention Center
Halls I, II, III

Molecular Probes and Fluorophores for Biological Imaging (#280)

Organized by: C. Fahmi, C. Cairo, C. Yip, Y. Horie

Poster Session

19:00 – 21:00

1594. New technology platforms to enable delivery of the immunoPET small molecule G-605. **D.E. Carrera***

1595. Development of dipolar dyes for two-photon imaging of tissues with suppressed autofluorescence. **H. Moon**, D. Kim, **C. Cho**, K. Ahn*

1596. Bioimaging of HER-2 specific affibody conjugated two-photon fluorescent probe for detection of breast cancer. **J. Choi**, C. Lim, D. Kang, B. Cho*

1597. Design and synthesis of a Gd(III) contrast agent that targets folate receptors. **M. Gil**, C.L. Molina, C.G. Gutierrez*

1598. Development of luminescent imaging probes for visualizing peroxynitrite. **M. Go**

1599. Janelia fluor dyes: Azetidinyl rhodamines as tunable bright fluorophores and caged dyes for live-cell and single-molecule microscopy. **J.B. Grimm**, A.K. Muthusamy, B.P. English, Z. Liu, W.R. Legant, J. Chen, J.P. Slaughter, R.H. Singer, T. Lionnet, L.D. Lewis*

1600. Two-photon dual-color imaging of mitochondria and lysosomes in live tissues. **S. Hong**, C. Lim, S. Ryu, D. Kang, B. Cho*

1601. Syntheses and characterisation of new fluorescent boron fluoride complexes. **A.C. Try***, **M. Howden**

1602. Detection of hydrogen sulfide by using two-photon excitable fluorescent probe. **S. singha**, **y. Jun**, **K. Ahn***

1603. Water soluble verdazyls as probes for biological systems. **D.J. Brook**, **T. Le**, **D. Matteo**, **H. Grewal**, **V. Changcoco**, V. Truong

1604. Development of activity-based probes for imaging human α -L-fucosidases in cells. **L. Lo***, Y. Hsu, M. Nandakumar, C. Lin

1605. Synthesis of Gd-MRI contrast agents bearing TTTA ligands and their structure-MRI properties relationship. **Y. Makita***, S. Fujiwara, A. Ogawa

1606. Long wavelength fluorescent probe for a highly sensitive quick detection of ascorbic acid. **Y. Matsukawa***, K. Ohkubo, T. Yamasaki, S. Fukuzumi, K. Yamada

1607. Mitochondrial selective efficient two-photon induced fluorescent probes possessing alkyli pyridinium group. **H. Morimoto**, A. Fujii, T. Shiraiishi, K. Satomi, H. Sugihara, Y. Suzuki, J. Kawamata*

1608. Fluorogenic, hypoxic-activated pro-drug strategy for targeted compound delivery and imaging. **L.J. O'Connor**, E.M. Hammond, S.J. Conway

1609. General labeling method of cell surface via azaelectrocyclization. **A. Ogura**, K. Tanaka*

1610. Synthesis and properties of photoreactive molecule localizing to organelles of living cell. **M. Ozaki***

1611. Ratiometric detection and imaging of biotools with BODIPY-based fluorescent probes. **D. Ma**, **H. Ryu**, K. Ahn*

1612. Two-photon fluorescent probes for detection of nucleus and mitochondria in human colon tissues. **C. Lim**, **S. Ryu**, D. Kang, B. Cho*

1613. Development of molecular probes for ¹⁹F NMR/fluorescence bimodal detection of DNAs in living cells. **T. Sakamoto***, D. Hasegawa, K. Fujimoto*

1614. Induction, detection, and mechanistic study of cell death induced by luminescent tris-cyclometalated iridium(III) complex-peptide hybrids. **N. Suzuki**, Y. Hisamatsu, A. Shibuya, H. Tanaka, A. Masum, S. Aoki

1615. Novel lysine-linked anthracenophanes used as cellular imaging agents to discriminate cancer cells from normal cells. **K. Takimoto***, Y. Kitayama, T. Takeuchi

1616. Novel azofluorescein for selective detection of zinc ion. **P. Thongyoog***, N. Choengchan, K. Chantalachana

1617. In-silico rule-based models for design of fluorophores. **Y.J. Tseng**, B. Su*, Y. Tu, O. Lin, Y. Harn, M. Shen

1618. Naphthalimide-based fluorescent probe for highly selective and sensitive detection of cadmium ions. **K. Tsukamoto***, S. Shimabukuro, H. Maeda

1619. Investigations of 2,7-diaminonaphthyridine conjugates for monitoring the hairpin probe PCR. **R.K. Verma**, F. Takei, K. NAKATANI*

1620. Probing the activation of T-cells by analogs of (E)-4-hydroxy-3-methyl-but-2-enyl diphosphate and their prodrugs. **R.R. Shippy**, D.P. Stockdale, A.M. Kilcollins, J. Li, C.C. Hsiao, R.J. Barney, A.J. Wiemer, **D.F. Wiemer***

1621. Labeling oligonucleotides and carbohydrates with BODIPY fluorophores. **T. Yan***, R. Yalagala, L. Yang, K. Tram

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

New Organosulfur Chemistry (#436)

Organized by: E. Block, E. Juaristi, A. Schwan, X. Jiang, C. Lee
Presiding: E.L. Clennan, C. Lee

19:00 – 1622. Sulfur atom tTransfer (SAT) reaction. **X. Jiang**

19:25 – 1623. Fluorinated hypervalent sulfur compounds. **J.T. Welch***, P.R. Savoie, L. Zhong, C.N. von Hahmann

19:50 – 1624. Computational studies of sulfur incorporation into poly(hexahydrotriazine) (PHT) rings. **G.O. Jones**

20:10 – 1625. Recent advances in the study of the anomeric effect with second-row elements sulfur and phosphorus. **E. Juaristi***, R. Notario*

20:35 – 1626. Recent developments in the sulfination of (hetero)aromatic rings: Direct access to sulfones and sulfonamides of medicinal chemistry relevance. **V. Mascitti***

* Principle Author

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Friday Morning

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25)

Organized by: T. Kubo, Y. Tobe,
M. Haley, G. Bodwell, K. Wong
Presiding: Y. Tobe

8:00 – 1627. Mathematical control in the self-assembly of giant M_1L_{2n} polyhedra.
M. Fujita*

8:40 – 1628. Bottom-up organic synthesis of carbon nanotubes.
R. Jasti*

9:05 – 1629. Adding multiple electrons to π -bowls: Structural outcomes.
M.A. Petrukhina*

9:30 – 1630. Multi-interactive azaphenalenenes.
Y. Yakiyama, J. Koo, G. Lee,
M. Kawano*

9:45 – 1631. Extended yet disjointed π -conjugation: Shape-dependent electronic properties of strings, branches, and macrocycles.
D. Lee*, K. Seyoung, M. Lee,
S. Kim

10:00 – 1632. Controlling the spacings separating adjacent aromatic linkers in ladder-phanes.
T. Luh

10:40 – 1633. (2,11)Teropyrenophanes as springboards to nanographenophanes.
G.J. Bodwell*, K. Unikela,
P. Ghods Ghasemabadi

11:05 – 1634. Novel fluorenyl-based hydrocarbon radicals.
T. Kubo*

11:30 – 1635. Optically active conjugated compounds based on planar chiral [2,2]paracyclophane.
Y. Morisaki*

11:45 – 1636. Probing electron transfer in the NapBox⁴⁺ family.
K.R. Hermann,
R. Young, J. Stoddart*

Hilton Hawaiian Village
Kalia Tower, Lehua Suite

Chemistry of Nanocarbons: Fullerenes, Carbon Nanotubes, Nanographenes and Related Materials (#41)

Organized by: T. Akasaka, F. Wudl,
L. Echegoyen, X. Lu, C. Wang
Presiding: A.L. Balch, T. Torres

8:00 – 1637. Searching for fullerene electron conductors for perovskite solar cells.
S. Xie*, S. Dai, L. Deng, C. Tian,
M. Zhang, R. Huang, L. Zheng

8:40 – 1638. Modification of work function of graphene by functionalization.
F. Lang, M. Barrejon*, M. Gomez-Escalona,
A.M. Rodriguez, J.R. Carrillo, M. Prieto

9:10 – 1639. Nanocarbons for optoelectronic applications.
D.M. Guld

9:40 – 1640. Syntheses of π -conjugated tubes and cages and their properties.
S. Yamago

10:00 – 1641. Functionalization of exfoliated graphene with electron donors.
N. Tagmatarchis*

10:20 – 1642. Synthesis, isolation, and crystallographic characterization of oxide clusterfullerenes $Sc_2O@C_{2n}$ ($n=38-41$).
N. Chen*, L. Feng*, T. Yang, Y. Hao,
Q. Tang

10:35 – 1643. Cluster vs. exohedral addend controlled Prato additions to endohedral metallofullerenes.
S. Osuna, M. Garcia Borrás, M.R. Cerón,
Y. Yamakoshi, L. Echegoyen

10:50 – 1644. Fullerene supramolecular assemblies.
A.L. Balch*, A. Aghabali,
M.M. Olmstead

11:20 – 1645. Uranium-based endohedral fullerenes.
L. Echegoyen*

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Natural Product-based Drug Discovery (#66)

Organized by: B. Baker, R. Kerr, Y. Qin,
D. Uemura, B. Littlefield
Presiding: T. Eguchi, B. Moore

8:00 – 1646. Characterization of monoclonal antibodies against the toxic turn of amyloid β 42 and their application to diagnosis for Alzheimer's disease.
K. Murakami*, M. Hanaki, M.L. Moro,
G. Giaccone, F. Tagliavini, K. Akagi,
R. Ishii, T. Tokuda, M. Maeda, N. Izuo,
T. Shimizu, K. Irie

8:30 – 1647. Biosynthesis of Aminoglycoside antibiotics.
T. Eguchi*

9:00 – 1648. Elucidation of pyranorignin biosynthetic pathway reveals mechanism of fused π -pyrone, exo-methylene and spiral cyclobutane formation.
K. Watabane*

9:40 – 1649. Developing next generation antibiotics and discovery tools.
B. Moore*

10:20 – 1650. Incorporating biosynthetic starting materials with rational drug design to optimize natural product drug leads for the control of cancer.
M.T. Hamann

10:50 – 1651. Fatty chemicals – a candidate for a new family of plant hormones and for a new agrochemical.
H. Kawagishi

11:20 – 1652. Patacamine analog developments for inhibition of translation initiation.
P. Teesdale-Spitte, H. Cumming,
J.E. Harvey

11:30 – 1653. Phytochemical investigation of northern Quebec lichens.
C. Carpenter*, N. Voyer, E. Ferreira-Queiroz,
J. Wolfender, M. Cuendet

11:40 – 1654. Novel bioactive natural products from medicinally important plants.
A. Ata*

11:50 – 1655. Total synthesis and structure-activity relationship of geranyl resorcylates derived from *Hericium erinaceum*, an edible mushroom with an antidementia effect.
S. Kobayashi*, K. Nagai

Hilton Hawaiian Village
Tapa Tower, Iolani Suite 1 & 2

Molecular Containers (#99)

Organized by: S. Mitsuhiro, L. Isaacs,
H. Yang
Presiding: R. Hooley, M. Yoshizawa

8:00 – 1656. Molecular containers based on functionalized calixpyrroles.
J.L. Sessler*

8:30 – 1657. Guest sequestration, packing, and folding within water-soluble nanocapsules.
B. Gibb

9:00 – 1658. Nanostructures prepared from self-assembly of pillararene-based amphiphiles and supra-amphiphiles.
F. Huang*, G. Yu, Y. Yao

9:25 – 1659. Gated molecular recognition and reactivity.
J. Badic

9:50 – 1660. Reversible structural transformations of nanocavities in crystalline peptide Ni(II)-macrocycles and their effects on adsorption behaviors.
R. Miyake*, C. Kuwata, Y. Masumoto,
M. Shionoya

10:10 coffee break

10:20 – 1661. Application of cucurbit[n]urils to the separation and sensing of proteins and the control of enzymatic catalysis.
W. Li, L. Smith, O. Ali, L.A. Losgdon,
A. Urbach*

10:40 – 1662. Synthesis and applications of mechanically chiral rotaxanes.
S. Goldup

11:00 – 1663. Dual host approaches to salt and amino acid transport.
P. Gale

11:30 – 1664. Biomedical applications of acyclic cucurbit[n]uril type receptors.
L. Isaacs*

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

Organoboron Chemistry: Applications in Organic Synthesis, Biology, and Materials (#100)

Organized by: D. Hall, B. Wang,
P. Duggan, M. Sugimura
Presiding: P. Duggan

8:00 – 1665. Novel molecular transformations based on catalytic activation of boron-containing σ -bonds by transition metals or 4,4'-bipyridines.
T. Ohmura*

8:30 – 1666. Application of lithiation-borylation methodology to the synthesis of natural products.
C. Brown*, V.K. Aggarwal

8:50 – 1667. Enantioselective allylboration of ketones using allylboronic acids.
R. Alam*, T. Vollgraff, K.J. Szabo

9:10 – 1668. Boronic acids as catalytic activators of (hetero)benzilic and allylic alcohols: More than simple Lewis acids.
A. McCubbin*

9:30 – 1669. Elucidation of Diels-Alder reactions of unsaturated boronic esters: Rational design, development, and mechanistic studies using experimental and computational methodologies.
N. Grimblat, M.M. Vallesjos, **S.C. Pellegrinet***

9:50 Break

10:00 – 1670. Development of a rapid assay for measuring gut permeability by recognition of biomarkers via a fluorescent probe based on boronic acids.
A. Resendez, B. Singaram*, D. Webb

10:20 – 1671. Facile amidination reaction of 2-aminoethylboronic acid for development of carbohydrate receptors.
B.B. Pappin, T. Garget, P.C. Healy,
M. Kiefel, T.A. Houston*

10:40 – 1672. Boronate-based pyrophosphate-specific molecular recognitions.
D. Iizuka, M. Sanjoh, T. Goda,
A. Matsumoto, Y. Miyahara

11:00 – 1673. Boron-containing compounds in drug discovery and chemical biology.
J. Zhang, F. Yang, **H. Zhou***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Recent Trends in Organocatalysis (#122)

Organized by: M. Terada, M. Shi,
J. Antilla, K. Maruoka

Presiding: J. Antilla, L. Deng,

Y. Iwabuchi, T. Ooi

8:00 – 1674. Asymmetric trienamine catalysis.
Y. Chen*

8:30 – 1675. Anion-recognition/ion-pairing approaches to asymmetric catalysis.
D. Seidel*

9:00 – 1676. Design and applications of organic ion-pair catalysts.
T. Ooi*

9:30 – 1677. Activation of nucleophiles for asymmetric reactions with organic molecules.
L. Deng*

10:00 – 1678. Asymmetric organocatalysis combined with metal catalysis: From concept to a general strategy.
L. Gong*

10:30 – 1679. New developments in asymmetric catalysis: Phosphoro-boronate mediated reactions.
J. Antilla*

11:00 – 1680. Selective functionalization of aromatics and heteroaromatics using organocatalytic systems.
Y. Kondo*

11:30 – 1681. Catalytic asymmetric oxidation using organocatalysts.
H. Yamamoto*

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Organic Reactions in Aqueous Media (#131)

Organized by: S. Kobayashi, B. Lipshutz,
C. Cai
Presiding: C. Cai, S. Kobayashi

8:00 Break

8:30 Opening Remarks

8:35 – 1682. Organic reactions in water different from organic reactions in organic solvents.
S. Kobayashi

9:00 – 1683. Barbier-Grignard reaction of aldehydes with aromatic halides in water.
C. Li*, F. Zhou

9:30 – 1684. Palladium-catalyzed conjugate addition of arylboronic acids to β,β -disubstituted enones on water: Improving reactivity to enable the synthesis of diaryl-substituted, quaternary stereogenic centers.
L.M. Stanley

9:50 – 1685. Lanthanide-promoted aqueous monoacetylation of diols by acyl phosphate monoesters on the way to unnaturally aminoacylated tRNA.
R. Kluger*, Y. Li

10:10 Break

10:25 – 1686. Molecular architecture-based administration of catalysis in water via self-assembly of an amphiphilic palladium pincer complex.
Y. Uozumi

10:55 – 1687. Expansion of bioorthogonal space: Development of biocompatible reactions with new functionalities.
J. Kim, C.R. Bertozzi*

11:15 – 1688. Micelle catalytic performance of newly designed surfactants based on Guerbet alcohols.
W. Dong*, J. Li

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Applications of C-H Functionalization (#169)

Organized by: P. Vachal, Z. Shi, C. Li,
H. Davies, K. Itami, H. Lebel

8:00 – 1689. Tunable, catalyst-controlled chemo- and site-selective nitrene transfer reactions.
J.M. Schomaker*

8:30 – 1690. Phosphine-cross-linked polystyrenes as platforms for producing C-H functionalization catalysts.
M. Sawamura*

9:00 – 1691. Understanding of aerobic oxidation α -triazole/acetophenone by copper(II) acetate.
H. Cha*, D. Chi

9:20 – 1692. Selective functionalization of C-H bonds with main group reagents.
J.F. Hartwig*

9:50 – 1693. Manganese-catalyzed C-C bond formation from inert C–H bonds.
C. Wang

10:10 – 1694. Ligand development in Rh(III) catalysis for C–H activation.
T. Rovis*

10:40 – 1695. Cross-dehydrogenative-coupling: From chemical synthesis to energy applications.
C. Li*

11:10 – 1696. Novel Cu-catalyzed oxidative C(sp³)–H bond functionalization–ring expansion tandem reactions.
O. Garcia Mancheno*

11:30 – 1697. C–H bond functionalization based on metal carbene migratory insertion.
J. Wang

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Strategies and Tactics for Complex Molecule Synthesis (#174)

Organized by: C. Forsyth, C. Lee,
L. Barriault, J. Cha
Presiding: C. Forsyth, S.E. Reisman

8:00 Introduction

8:05 – 1698. Concise synthesis of diterpenes via gold catalyzed processes: From complexity to simplicity.
L. Barriault*, G. Bellavance, P. McGee, A. Canillo

8:35 – 1699. Function- and diversity-driven total synthesis of natural products.
M. Dai*

9:05 – 1700. Nitramines as reagents for complex molecule construction.
A.E. Mattson

9:35 break

9:40 – 1701. Cascade approach to the total synthesis of virosaine.
J. Gleason, J. Hughes

10:00 – 1702. Diversity-oriented synthesis of *Streptomyces* antibiotic natural products.
J.H. George

10:15 – 1703. Bioinspired platform for the synthesis of lignan natural products.
J. Lumb*, A. Albertson

* Principle Author

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10:35 – 1704. General route to antifeedant sesterpenoids: Enantioselective synthesis of leucosceptrid natural products. **T. Magauer***, C.L. Hugelshofer
10:55 break
11:00 – 1705. Catalytic methods for simplifying synthesis. **D.J. Dixon***
11:30 – 1706. Catalytic approach to the synthesis of novel natural products. **C. Lee**

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Molecular Probes and Fluorophores for Biological Imaging (#280)

Organized by: C. Fahrni, C. Cairo, C. Yip, Y. Hori
Presiding: C.M. Yip

8:00 Opening Remarks

8:05 – 1707. Cyanine fluorophores: From two-photon imaging to inhibition of amyloid peptide aggregation. **M. Wong***, L. Guo, D. Xu, S. Ho, H. Li

8:25 – 1708. Fluorescent labeling strategies for phospholipids and cellular glycans. **C. Cairo**

8:55 – 1709. From chemoselective fluorescence imaging of ROS to controlled delivery of cytotoxic agents enabled by activatable probes. **G. Costa***

9:25 – 1710. Red fluorescent proteinaceous probes for visualization of neuronal activity. **R.E. Campbell**

9:55 Session Break

10:10 – 1711. Molecular probes for continuous monitoring of ATP/ADP ratio. **V. Pierre**

10:40 – 1712. Tailored zwitterionic near-infrared fluorescent contrast agents for in vivo imaging. **M. Henary***, E. Owens, H. Choi

11:10 – 1713. Development of far-red to near-Infrared fluorophores and their application to fluorescence probes to detect hypoxia *in vivo*. **K. Hanaoka***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Organic Solid-State Chemistry: Structure, Property & Reactivity (#398)

Organized by: M. Sakamoto, L. MacGillivray, J. Vittal
Presiding: N. TOHNAlJ, J.J. VITALL

8:00 – 1714. Nonporous but yet gas-sorbing molecular crystals. **H. Tsue***, H. Takahashi, R. Tamura

8:20 – 1715. Nanoporous materials for confined polymerization and molecular rotor dynamics. **P. Sozzani***, S. Bracco, M. Forani, D. Piga, A. Comotti

8:40 – 1716. Crystal crosslinking method: The third kind of crystalline polymerization. **K. Kokado***, T. Ishiwata, Y. Furukawa, K. Sada*

9:00 – 1717. Single-crystal-to-single-crystal transformation of metallosupramolecules with cyclic and acyclic thioethers. **S. Lee***

9:30 – 1718. Insight into the formation of covalent organic frameworks. **W. Dichtel**

10:00 break

10:10 – 1719. Molecular materials exhibiting zero-dimensional pores. **K.T. Holman***

10:40 – 1720. Formation, transformation of organic crystals, and the characterization. **R. Kuroda***

11:10 – 1721. Solid-state properties of CB⁻PQT⁴⁺, CBPQT^{2(•+)}, CBPQT⁰, and catenanes containing these different redox states of CBPQT⁴⁺. Z. Liu, M. Frasconi, I. Fernando, **J.F. Stoddart**

11:40 – 1722. Crystal engineering: Solid-state reactivity via principles of supramolecular chemistry. **L.R. MacGillivray**

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

New Organosulfur Chemistry (#436)

Organized by: E. Block, E. Juaristi, A. Schwan, X. Jiang, C. Lee
Presiding: X. Jiang, W. Weigand

8:00 – 1723. Transition-metal-catalyzed C-S bond cross-coupling reaction. **C. Lee**
8:30 – 1724. Design and synthesis of chiral oxathiazinone scaffolds: Efficient synthesis of hindered enantiopure sulfonamides and their applications to chiral amine synthesis. **C. Senanayake**

9:25 – 1725. Smelling sulfur. **E. Block***, H. Zhang

9:50 – 1727. Sulfur mediated allylic C-H alkylation reaction. **P. Li***

10:10 Break

10:20 – 1728. Synthesis of 3,3'-diaryl-1,1'-binaphthalene-2,2'-disulfonic acids and design of chiral 3,3'-Ar₂-BINSA salt catalysts. **K. Ishihara***, M. Hatano, K. Nishikawa

10:40 – 1729. Palladium-catalyzed C-S bond activation of alpha-oxo ketene dithioacetals for C-C couplings: Construction of carbo- and heterocyclic compounds. **M. Wang**, J. Chang, Y. Yang, P. Chen

11:05 – 1730. Journey from discovery of new extended Pummerer chemistry to catalytic C-S bond cleavage. **H. Yorimitsu***

11:30 – 1731. Asymmetric sulfa-Michael reaction: Catalysis by an iron(III) complex. **S. Shaw***, J. White

11:55 Closing Remarks by Eric Block

Friday Afternoon

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25)

Organized by: T. Kubo, Y. Tobe, M. Haley, G. Bodwell, K. Wong
Presiding: G.J. Bodwell

13:00 – 1732. From azapentacenes to aza-heptacenes - synthesis, properties, and applications. **U. Bunz***, J. Engelhart, P. Biegger, F. Paulus

13:40 – 1733. Synthesis and properties of imide derivatives with polycyclic conjugated systems involving five-membered ring systems. **T. Kawase**

14:05 – 1734. Zethrene, its substituted and π-extended derivatives: Synthesis, structural analysis, and properties. **Y. Wu**

14:30 – 1735. Benzobisoxazole cruciforms: New tunable cross-conjugated materials for organic electronics. **M. Jeffries-EL**, R. Chavez, A. Burney-Allen, B. Tlach, A.L. Tomlinson

14:45 – 1736. Synthesis and complexation with C₆₀ of electron-donating triacalix[n]dithiophene. **M. Hasegawa***, R. Inoue, Y. Honda, Y. Mazaki

15:00 – 1737. Functionalized acenes in organic electronics. **J. Anthony**

15:40 – 1738. Boron cations and poly-dentate divalent group 14 ligands. **C. Chiu**

16:05 – 1739. From nonplanar polycyclic arenes to carbon-rich materials. **Q. Mao***, K. Cheung, L. Shan, X. Gu

16:30 – 1740. *Prototeroisomerization* of Nindigo: Mechanistic and spectroscopic studies of the acid/base chemistry. **E.C. Nicholls-Alison**, G. Nawn, R. Hicks, B. Patrick

16:45 – 1741. Fluorescence enhancement of covalently linked fluorescent chromophores with naphthalene-1,8-diy linker units: Analysis based on kinetic constants. **T. Hirose**, Y. Tsuno, Y. Fujimori, K. Matsuda*

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Anion Receptors (#31)

Organized by: B. Hay, F. Pfeffer, B. Wu, C. Jia, R. Custelcean
Presiding: M. Albrecht, B. Hay

13:00 Opening Remarks

13:05 – 1742. Anion recognition with shape persistent macrocycles. **A. Flood***

13:35 – 1743. Anion receptors based on triazole-containing cyclic pseudopeptides. **S. Kubik***, D. Mungalpara

14:05 – 1744. Steroid-inspired transmembrane anion carriers. **A. Davis***

14:35 – 1745. Arylacetylenes as modular scaffolds for anion recognition: Water-soluble hosts and insights into aryl CH₃•X⁻ hydrogen bonds. **B.W. Tresca**, R.J. Hansen, M.M. Haley, **D.W. Johnson**

15:05 Break

15:20 – 1746. Molecular recognition of anionic cell surfaces using Zn-DPA complexes. **B. Smith***

15:50 – 1747. Anion recognition by silanol-based receptors. **S. Kondo**

16:20 – 1748. Extending the reach of polynorbornane based hosts for anions. **F.M. Pfeffer***, R. Robson, J.R. Engstrom, L. O'Dell

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Natural Product-based Drug Discovery (#66)

Organized by: B. Baker, R. Kerr, Y. Qin, D. Uemura, B. Littlefield
Presiding: S. Band Horwitz, M. Uesugi

13:00 – 1749. Natural products: An opportunity for discovery in chemistry and biology. **J.K. De Brabander***, W. Li

13:40 – 1750. Small molecule tools for cell biology and cell therapy. **M. Uesugi**

14:20 – 1751. Taxol®, tubulin and tumors. **S. Band Horwitz***

15:00 – 1752. Endogenous nitrated nucleotide is an autophagy inducer. **H. Arimoto***

15:20 – 1753. Synthesis of acylquinic acids and their functional studies toward drug discovery. **K. Yoshida***, K. Oyama, T. Yamada, T. Kondo

15:40 – 1754. Marine hydroquinone zonarol prevents inflammation and apoptosis in dextran sulfate sodium-induced mice ulcerative colitis. **T. Koyama***, S. Yamada, T. Sato

16:00 – 1755. Natural product derivatives with potent and selective activity vs. fluoroquinolone-resistant pathogens. **P.J. Hergenrother**

16:10 – 1756. Acalutane and toddaculin from *Toddalia asiatica* (L.) Lam. suppress lipopolysaccharide induced inflammation of RAW264 macrophages through different modes of action. **M. Kumagai**,

A. Watanabe, T. Mishima, I. Yoshida, K. Koizumi, M. Ide, K. Fujita, M. Watai, K. Nishikawa, Y. Morimoto

16:20 – 1757. Alkaloidal content of *Rauvolfia nukuhivaensis*: New inhibitory hERG channel compounds. **P. Raharivelomanana***, N. Martin, S. Fernandez-Ferreiro, F. Barbaud, M. Nicolas, G. Lecellier, C. Paetz, M. Gayssens, E. Alonso, O. Thomas, L. Botana

16:30 – 1758. Synthetic and biomechanistic investigations of agelastatin A. **M. Jouanneau**, B. McClary, J.O. Liu, D. Romo*

16:40 – 1759. Isolation of tomurilane, a novel thiazole containing polyketide with selective cytotoxicity under glucose-restricted conditions. **O. Ohno***, K. Same, C. Kudo, S. Sumimoto, T. Teruya, E. Tashiro, S. Simizu, M. Imoto, K. Suenaga

16:50 – 1760. Duocarmycins to nitroCBIs: From toxic DNA alkylators to hypoxia-selective antitumor agents. **M. Tercel***, F.B. Pruijn*, R.J. Stevenson, S.P. McManaway, H.S. Liyanage, H.H. Lee, A. Ashoorzadeh, P. O'Connor, S.Y. Mehta

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

13:00 – 1761. Allylboronic acids in organic synthesis. **K.J. Szabo***

13:30 – 1762. Pd-catalyzed sequential arylation of methyl sulfone derivatives toward straightforward synthesis of di- and tri-arylmethanes. **M. Nambo***, E.C. Keske, J.P. Rygus, C. Cruden

13:50 – 1763. Enantioselective borylation dearomatization of indoles by copper(I) catalysis. **K. Kubota***, K. Hayama, H. Iwamoto, H. Ito*

14:10 – 1764. 1,1-Carboboration route to phospholes - mechanistic insight and applications. **J. Mabus***, G. Erker

14:30 – 1765. Combination of boron and C₁ chemistries at transition metal centers. **A.F. Hill***, J.S. Ward, R. Shang, C.D. Stewart

14:50 Break

15:00 – 1766. α-Boryl aldoximes: Novel reagents for the synthesis of drug-like small molecules. **S.K. Liew**, A.K. Yudin*

15:20 – 1767. Novel routes to boron allylation reagents derived from propargyl esters. **R. Melen***

15:40 – 1768. Facile preparation of aryne-nickel complexes from *ortho*-borylaryli triflates and their synthetic applications. **Y. Sumida**, T. Sumida, T. Hosoya

16:00 – 1769. Stereoselective preparation of 2,3,3-triarylacrylic acid esters using Suzuki-Miyaura coupling reactions. **S. Cardinal**, N. Voyer*

16:20 – 1770. Cross-coupling and addition reactions of trifluoromethyltrialboreate salt. **Y. Yamamoto***

Hilton Hawaiian Village
Mid-Pacific Center, Coral 4

Recent Trends in Organocatalysis (#122)

Organized by: M. Terada, M. Shi,

J. Antilla, K. Maruoka

Presiding: Y. Hayashi, Y. Kita, L. Kurti, M. Terada

13:00 – 1771. Toward new activation modes via carbene organocatalysis. **Y. Chi***

13:30 – 1772. Pushing the limits of organocatalysis: Enantioselective transformations of α-branched ketones. **S. Luo***

14:00 – 1773. Metal-free oxidative biaryl coupling reactions by hypervalent iodine reagent. **Y. Kita**

14:30 – 1774. Amidine-based catalysts and their applications in enantioselective acyl transfer. **V. Birman***

15:00 – 1775. Enantioselective transformation of cationic intermediates mediated by chiral phosphoric acid catalyst. **M. Terada***

15:30 – 1776. Atroposelective synthesis of functionalized biaryls. **L. Kurti***

16:00 – 1777. Pot-economy and organocatalysis in total synthesis. **Y. Hayashi***

16:30 – 1778. Anion-binding catalysis. **E.N. Jacobsen***

Hilton Hawaiian Village
Kalia Tower, Hibiscus 2

Organic Reactions in Aqueous Media (#131)

Organized by: S. Kobayashi, B. Lipshutz, C. Cai

Presiding: S. Kobayashi, B.H. Lipshutz

* Principle Author

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13:00 – 1779. Chemistry in water using micelles: Applications in the pharmaceutical industry. **W.M. Bräfe***

13:30 – 1780. Copper-catalyzed borylation and silylation reactions in water. **W.L. Santos**

14:00 – 1781. Sustainable gold catalysis in water. **N. Krause***

14:20 – 1782. Multicomponent and palladium-catalyzed coupling reactions in aqueous media. **C. Cai**

14:50 Break

15:05 – 1783. Ruthenium catalyzed C-H bond functionalization in water. **P.H. Dixneuf*, F. Pozgan, P.B. Arockiam, B. Li, K.S. Devavaraj, K.S. Singh**

15:35 – 1784. Organic reactions with strong acids: Role of water as acid switch from Lewis acid to Bronsted acid, solvent and reagent. **P. Prakash, T. Mathew*, P.A. Olah**

15:55 – 1785. Reactivity of pyrite and dazomet, a hydraulic fracturing additive. **N. Consolazio, G. Lowry, A. Karamalidis**

16:15 – 1786. Transitioning organic synthesis from organic solvents to water. **B.H. Lipshutz***

16:45 Closing Remarks

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Applications of C-H Functionalization (#169)

Organized by: P. Vachal, Z. Shi, C. Li, H. Davies, K. Itami, H. Lebel

13:00 – 1787. Transition metal-mediated direct couplings on heteroarenes. **M. Miura***

13:30 – 1788. Advances, challenges, and opportunities for direct C-H bond functionalization in materials chemistry. **S.R. Marder, J. Zhang, A. Rojas, T. Parker, S.B. Blakey, Q. Shi, C.N. Scott**

14:00 – 1789. Direct arylation polymerization synthesis of a series of new silole-benzazole copolymers. **C.N. Scott*, M. Bisen**

14:20 – 1790. Direct transformation of unreactive C-H bonds. **Z. Shi***

14:50 – 1791. Hydrogen bond-controlled meta-selective C-H borylation of aromatic compounds. **Y. Kuninobu*, H. Ida, M. Nishi, M. Kanai***

15:10 – 1792. Asymmetric C-H bond functionalizations: A quest for efficient ligand systems. **N. Cramer***

15:40 – 1793. Stereoselective C-H aminations. **H. Lebel*, J. Bartholoméus, M. Khalifa**

16:10 – 1794. Development of transition-metal-catalyzed imidation for adding handles to functional molecules. **K. Murakami, T. Kawakami, K. Itami***

16:30 – 1795. Ligand-accelerated C-H activation reactions: Near and far. **J. Yu***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Strategies and Tactics for Complex Molecule Synthesis (#174)

Organized by: C. Forsyth, C. Lee, L. Barriault, J. Cha
Presiding: C. Lee, L. Xiao

13:00 Introduction

13:05 – 1796. New alkaloid synthesis by ring opening of functionalized cyclopropanols. **J.K. Cha**

13:35 – 1797. Adventures in unnatural and natural product synthesis. **M. Sherburn***

14:05 – 1798. Towards the synthesis of the brasiliolides using 1,5-*anti* selective aldol reactions. **M. Housden, C. Cordier, P. Burton, F. Muehlthau, I. Paterson**

14:25 – 1799. Synthetic studies on catechin-class polyphenols: Monomers and oligomers. **K. Suzuki, K. Ohmori**

14:50 break

14:55 – 1800. Synthetic studies on tetrodotoxin. **T. Fukuyama*, T. Maehara, K. Motoyama, T. Toma, S. Yokoshima**

15:25 – 1801. 1,2-Rearrangement reaction and its application to natural product synthesis. **Y. TU***

15:55 – 1802. Strategies for construction of the bis(indole) alkaloid isatines A and unnatural analogs via a dual catalysis process. **F. West***

16:25 – 1803. Asymmetric methods for the synthesis of pyran-based natural products. **T.E. Smith***

16:45 – 1804. Towards the synthesis of the macrolide glycoside biselyngbyaside. **L. Kaemmler, M.E. Maier***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Chemical Glycosylation: Methods and Mechanisms (#306)

Organized by: T. Lowary, X. Huang, S. Hung, K. Tanaka
Presiding: T. Lowary

13:00 – 1805. *N*-Glycosides with uses from protecting-group-free glycosidations to site-specific protein modifications. **M. Nitza**

13:30 – 1806. New methods and strategies for the glycan synthesis. **X. Li***

14:00 – 1807. One-pot glycan conjugation to protein via azaelectrocyclization: Dynamics analysis of neoglycoproteins in live animal. **A. Ogura, K. Tanaka***

14:15 – 1808. Partially unprotected *N*-acetyl sialyl donors undergoing α -sialylation without the nitrile effect. **T. Aoyagi, S. Ohira, S. Fuse, H. Tanaka***

14:30 – 1809. Stereodirecting participation from near and far. **D. Crich*, P. Wen, S. Dharuman**

15:00 Break

15:10 – 1810. Glycosylation using 3,6-O-(o-xylylene)-bridged glucosyl donor. **H. Yamada*, Y. Okada, N. Asakura, M. Bando, Y. Ashigara, A. Motoyama, A. Fukumoto, T. Arai**

15:40 – 1811. What is the origin of high stereoselectivity in the DTBS-directed α -galactosylation? **A. Imamura*, H. Ando, H. Ishida, M. Kiso***

15:55 – 1812. TMSOTf-catalyzed per-O-trimethylsilylation reaction for concise synthesis of glycoconjugates. **C. Wang**

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

New Horizon of Process Chemistry by Scalable Reactions and Technologies (#426)

Organized by: K. Tomioka, R. Williams, R. Hwu, H. Sajiki, T. Shioiri, N. Yasuda
Presiding: K. Tomioka

13:00 – 1813. Short step asymmetric synthesis of complex molecules. **K. Tomioka***

13:20 – 1814. Catalytic ruthenium carbenes: New modes of cyclization. **J.A. Varela*, F. Cambeiro, D. Padín, C. Saá***

13:40 – 1815. Efficient synthesis of pyrimidine derivative, CH5132799: Control of residual palladium and overall process optimization. **Y. Hosoya*, A. Kawase, K. Maeda, T. Ichige, M. Murakata**

13:55 – 1816. Dinuclear iron complex-catalyzed transesterification: Synthesis of *tert*-butyl esters and unprecedented chemoselectivity. **T. Ohshima*, R. Horikawa, C. Fujimoto, R. Yazaki**

14:15 – 1817. Development of the novel *kōkini peptide*. **Y. Tahara*, T. Ohsu, Y. Amino, H. Nagasaki, T. Yamamoto, S. Takeshita, T. Hatanaka, Y. Maruyama, M. Kaneko, M. Nakazawa, S. Suzuki, N. Miyamura, Y. Eto**

14:30 – 1818. Development of scalable synthesis and quality control strategy for ER-403812-09. **A. Kayano*, T. NAKAMURA, M. Matsuda, M. ISOMURA, K. YOSHIZAWA, M. OMORI, S. IWASHITA, T. KODERA, T. SASAKI, H. KUMOBAYASHI, Y. OKADA, K. TAGAMI, G. Moniz, J. Del Vecchio, F. Fang**

14:50 Break

15:00 – 1819. Design and analysis of a continuous gas-phase process for the production of hexafluoropropene oxide. **D. Lokhat*, M. Starzak, D. Ramjugernath**

15:15 – 1820. A challenging synthesis of the highly functionalized echinocandin ASP9726, a successor of micafungin: How can we achieve the large-scale synthesis?. **S. Yoshida***

15:35 – 1821. Vortex fluidic device – thin film processing technology gets a new spin. **J. Britton, C. Raston**

15:50 – 1822. Process development of GS-9669. **S. Fujimori**

16:10 – 1823. New horizon of lipase-catalyzed dynamic kinetic resolution of alcohols for producing optically active compounds. **S. Akai***

16:30 – 1824. Enabling sustainable organic synthesis via electrochemistry. **D.G. Blackmond*, A. OBrien, B. Rosen, O. Luca, P.S. Baran**

Hilton Hawaiian Village
Kalia Tower, Kahili 1 & 2

Synthetic Modulators of Protein-Protein Interactions (#461)

Organized by: P. Arora, D. Fairlie, A. Kennan, K. Kumar, S. Sidhu, ,
Presiding: K. Kumar

13:00 Opening Remarks

13:05 – 1825. Approaches to modulating protein-protein interactions. **D.P. Fairlie***

13:30 – 1826. New computational tools to target protein-protein interaction interfaces. **Y. Zhang***

13:50 – 1827. Allosteric modulators of the PD1-PDL1 interaction: Small molecule agonists and antagonists from a unified structural dynamics approach. **J.E. Wulff, R. Hanley**

14:10 Break

14:20 – 1828. Structure-based development of potent small molecule inhibitors of the menin-MLL interaction for cancer therapies. **D. Borkin, H. Miao, J. Pollock, T. Purohit, T. Cerpicki**

14:45 – 1829. Small molecules that induce influenza nucleoprotein oligomerization and inhibit virus replication *in vitro* and *in vivo*. **S.W. Gerritz, C. Cianci, S. Kim, B.C. Pearce**

15:10 – 1830. Structure based design of allosteric inhibitors of hypoxia inducible factor. **U.K. Tambar**

15:30 Break

15:40 – 1831. Discovery of small molecule inhibitors targeting the SUMO-SIM interaction using a protein interface consensus approach. **A.R. Voet, A. Ito, M. Hirohama, S. Matsuoka, N. Tochio, T. Kigawa, M. Yoshida, K. Zhang***

16:05 – 1832. Synthesis and structure function relationship study of fusicoxin/cotylenin analogs. **Y. Higuchi*, F. Yesil, T. Yoneyama, C. Ottmann, J. Ohkanda, N. Kato***

16:25 – 1833. Inhibition of MDM4-p53 interactions for retinoblastoma. **R. Guy***

Friday Evening

Hawaii Convention Center
Halls I, II, III

Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25)

Organized by: T. Kubo, Y. Tobe, M. Haley, G. Bodwell, K. Wong

Poster Session

19:00 – 21:00

1834. X-ray spectroscopic characterization of organic semiconductor nanowires. **A. Mazaheriour, N. Husken, J. Jocsón, G. Kladnik, A. Cossaro, L. Floreano, A. Verdini, A. Burke, K. Miller,**

A. Masurkar, J. Kymissis, D. Cvetko, A. Morgante, A.A. Gorodetsky

1835. Photochemical synthesis of phenacenes and acylphenacenes, and the optical properties studied by emission and transient absorption measurements. **M. Yamaji*, H. Okamoto**

1836. Recent progress in chemistry of subporphyrins. **A. Osuka***

1837. Synthesis, two-step equilibrium, and optical properties of fused dimeric rhodamine dyes with near-IR emission.

Y. Shirasaki*, A. Muranaka, S. Kamino, D. Hashizume, D. Sawada, M. Uchiyama

1838. Supramolecular interaction of fullerenes with a curved π -surface of a monomeric quadruply ring-fused porphyrin.

T. Ishizuka*, Y. Saegusa, T. Kojima, S. Mori, M. Kawano, T. Kojima

1839. Theoretical study on the optical response properties of molecular aggregates of open-shell polycyclic aromatic hydrocarbons. **R. Kishi*, M. Saito, N. Matsushita, K. Yoneda, M. NAKANO**

1840. Development of a dendritic donor-acceptor structure with potential gradient. **T. Heeger*, K. Albrecht, K. Yamamoto**

1841. Design and synthesis of pentacene-based acceptors for organic photovoltaics. **M. Gruber, A. Waterloo, A. Kunzmann, R. Casillas, R.D. Costa, D.M. Guldi, R.R. Tykwiński***

1842. Synthesis and properties of novel overcrowded quinone having various structures with close energies. **T. Suzuki*, T. Nishiuchi, Y. Hirao, T. Kubo**

1843. Photophysical and structural chemistry of 5-arylamino thiazoles as new pi-electron systems. **K. Yamaguchi*, T. Murai**

1844. Synthetic bacterioclorins – tunable molecules for capturing near-infrared light. **J. Lindsey***

1845. Syntheses and basic properties of tetraphienonaphthalene: Photoinduced electron-transfer cyclization–dehydrogenation reactions of tetra(3-thienyl)ethane. **A. Yamamoto, E. Ohta, Y. Matsui, K. Mizuno, H. Ikeda***

1846. Syntheses and crystallographic studies of an angularly-fused thienobis[1]benzothiophene and its CT cocrystal with TCNQ. **T. Ogaki*, A. Yamamoto, E. Ohta, Y. Matsui, K. Mizuno, H. Ikeda***

1847. Crystal structures of 4-diethylborylpyridine pentamer and hexamer. **S. Wakabayashi*, S. Komeda, Y. Shimizu, Y. Ohki, K. Tatsumi**

1848. Control of conformational isomers showing distinct colors for nitrogen-contained bis(tricyclic) aromatic ene. **T. Suzuki, H. Okada, T. Nakagawa, Y. Matsuo**

1849. Mechanochromic luminescence properties of D-A-D type dibenz[a,j]-phenazine derivatives. **M. Okazaki, Y. Takeda, S. Minakata**

1850. Synthesis and properties of acid- and base-responsive molecules containing conjugated phenolic substituents bridged by heterocycles. **T. Kawano*, T. OHASHI, H. MURAOKA, S. OGAWA**

1851. Synthesis and properties of zwitterionic singlet biradicaloid bisphenalenyl. **K. Furukawa, T. Nishiuchi, Y. Hirao, T. Kubo***

1852. Synthesis and property of carbazole-based BODIPYs. **T. Todaka, C. Maeda, T. Ema**

1853. Synthesis of carbazole-based porphyrins. **C. Maeda, M. Takata, A. Honsho, T. Ema**

1854. One-step synthesis of [16]helicene by multiple photocyclization. **T. Murase***

* Principle Author

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onlineprogram

- 1855.** 18 π -Electron tautomeric benzophthalocyanine: A functional near-infrared dye with tunable aromaticity. **N. Toriumi**, A. Muranaka*, K. Hirano, K. Yoshida, M. Uchiyama*
- 1856.** Syntheses and properties of trinaphtho[3,3,3]propellane based three-fold symmetric molecules aimed at construction of distinctive 2D honeycomb electronic structure. **T. Kodama**, T. Nishiuchi, Y. Hirao, T. Kubo*
- 1857.** Aryne polymerization: Straightforward synthesis of elusive poly(*ortho*-arylene)s. **Y. Mizukoshi**, K. Mikami*, M. Uchiyama*
- 1858.** Novel fluorocarbon-functionalized small molecules for organic field-effect and light-emitting transistors. **M.L. Denti**, H. Usta, W.C. Sheets, G. Generali, R. Capelli, S. Lu, X. Yu, M. Muccini, A. Faccetti
- 1859.** Structural characterization and luminescent properties of indolo[3,2-*b*]carbazoles. **M. Hirano**, T. Moriuchi, T. Hirao*
- 1860.** Metallocenes with sumanenyl ligand. **S. Kato**, T. Amaya, Y. Takahashi, T. Moriuchi, T. Hirao
- 1861.** Photochemical syntheses and photophysical studies of condensed coumarin derivatives that could be potential for blue emission and semiconductor devices. **Y. Hakoda**, H. Okamoto, M. Yamaji*
- 1862.** Toward the realization of “Molecular n-Bit Memory”: Preparation and dynamic redox behaviors of novel electron donors containing multiple dyreux units. **H. Tamooki**, R. Katoono, K. Fujiwara, T. Suzuki*
- 1863.** Synthesis and fluorescence properties of symmetric and asymmetric diazo[1,2-*a*:2',1'-*c*]quinoxaline derivatives in solution and in the solid state. **S. Matsumoto**, K. Sakamoto, E. Batmunkh, S. Qu, T. Kobayashi, M. Kamehiro, M. Akazome
- 1864.** Synthesis and investigation of unsymmetrically substituted [n]cumulenes. **M.U. Bühringer**, H. Maid, F. Hampel, R.R. Tykiewski*
- 1865.** Nonplanar *meso*-trifluoromethyl substituted β -octaalkylporphyrins. **M. Suzuki***, K. Okinaga, T. Hoshino, S. Neya, Y. Nishigaiwa
- 1866.** Theoretical investigation of open-shell singlet nature, aromaticity and nonlinear optical properties of π -conjugated condensed-ring systems involving antiaromatic rings. **K. Fukuda**, M. NAKANO
- 1867.** Phenalenyl-fused porphyrin biradicals. **Z. Wangdong**, J. Wu*
- 1868.** Structure-property relationships and applications of π -conjugated boron difluoride formazanate dyes. **S.M. Barbon**, J.B. Gilroy*
- 1869.** 20 π -Electron benzophthalocyanines: Reduced-symmetry antiaromatic porphyrinoids that exhibit intense near-infrared absorption. **S. Yanagi**, N. Toriumi, A. Muranaka*, M. Uchiyama*
- 1870.** Rh-catalyzed efficient synthesis for condensed polycyclic compounds by [2+2+2] cycloaddition of benzothiophene dioxides and α,ω -dienes. **Y. Tahara**, M. Gake, R. Matsubara, T. Shibata*
- 1871.** Synthesis and properties of acrylamide polymers having carbazole moieties. **K. Tani***, K. Hori, H. Takemura, K. Sakakibara, Y. Tsuji
- 1872.** Acid/base-regulated reversible electron transfer disproportionation of hydrazinohelicenes. **S. Higashibayashi***
- 1873.** Computational design of denzo-bisazole materials for use in organic electronics. **A.L. Tomlinson**, M. Jeffries-EL
- 1874.** Efficient synthesis of multisubstituted dibenzothiophene derivatives by catalytic [2+2+2] cycloaddition. **R. Matsubara**, Y. Tahara, T. Shibata*
- 1875.** Towards novel BODIPY cyclophanes for advanced materials applications. **B.A. Hussein**, B.D. Koivisto*
- 1876.** Synthesis of phenyl viologen type molecular wire toward construction of electrochemical responsible Au-nanoparticles network. **Y. Kobayashi**, K. Suzuki, T. Sugawara*
- 1877.** Structures and properties of bis(tri-oxyphenylamine) and its cationic species. **N. Tanaka**, S. Suzuki, M. Kozaki, K. OKADA*
- 1878.** Micromolding in capillaries for the fabrication of high performance of organic ambipolar field effect transistors. **S. Watanabe**, T. Fujita, T. Aoyama, J. Riviere, M. Uchiyama, M. Matsumoto
- 1879.** Conversion of 2-iodobiaryl to 2,2'-diiodobiaryl via oxidation–iodination sequences: A versatile route to ladder-type heterofluorenes. **B. Wu**, N. Yoshikai*
- 1880.** Bottom-up synthesis of highly soluble and very narrow armchair edge graphene nanoribbons. **W. Yang**, W.A. Chalifoux
- 1881.** Proton-mediated chromatic system of octaethylporphyrin derivatives with highly sensitive, stable, and dramatic behaviors in their spectral changes. **H. Kempe**, J. Yamamoto, M. Ishida, J. Yoshino, N. Hayashi, H. Higuchi*
- 1882.** Studies on syntheses and properties of open-shell molecular system ligated with pi-conjugated phosphines. **S. Kira**, S. Suzuki, M. Kozaki, K. OKADA*
- 1883.** Theoretical study on open-shell singlet nature and nonlinear optical properties of π -stacked thiacyl radical multimers. **H. Matsui**, K. Fukuda, K. Yoneda, M. NAKANO*
- 1884.** Convenient synthesis of benzocarbazole derivatives and evaluation of organic EL property. **C. Akazaki***, H. Nishino
- 1885.** Synthesis of the new cyclobutadiene derivatives by photoisomerization of tetrahedrane. **Y. Kobayashi**, M. Nakamoto, A. Sekiguchi*
- 1886.** Synthesis of substituted thiophene-containing multicyclic compounds by intramolecular [2+2+2] cycloaddition. **S. Kitा**, T. Shibata*
- 1887.** Direct mono- and difunctionalization of perlyenediimides. **F. Fernandez-Lazaro***, N. Zink-Lorre, D. Gutierrez-Moreno, E. Font-Sanchis, Á. Sanchez-Santos
- 1888.** Synthesis of twisted PAHs by cyclization of bis(10-aryl/naphthalene-9-yl) substituted benzenes or naphthalenes. **A. Oishi**, Y. Tokoro
- 1889.** Theoretical study on singlet fission in polyaromatic hydrocarbon dimers: Electronic and vibronic coupling. **S. Ito**, M. NAKANO*
- 1890.** Dithiaquinoidal-[n]thienoacenes with biradical character. **X. Shi**, C. Chi*
- 1891.** Self-assembled conjugated polymer microspherical optical resonators. **Y. Yamamoto***, K. Tabata, D. Braam, S. Kushida, J. Kuwabara, T. Kanbara, A. Lorké
- 1892.** Allosteric inhibition of the ligand-binding ability of zinc porphyrin using the regulatory molecule. **Y. Sasaki**, M. Kozaki*, S. Suzuki, K. OKADA
- 1893.** Chirality and fluorescent properties of photochromic pirazine-annulated dihydropyrene. **T. Sawada***[†], S. KUBO, K. Nanamura
- 1894.** π -Electronic systems that provide various anion complexes and resulting ion-pairing assemblies. **R. Yamakado**, H. Maeda*
- 1895.** Syntheses and properties of metal salen complexes for dye sensitized solar cells. **Y. Ueda**, S. Suzuki, M. Kozaki, K. Iso, A. Konno, K. OKADA*
- 1896.** Synthesis and properties of azulene-fused polycyclic aromatic hydrocarbons. **M. Murai***, S. Iba, K. Takai*
- 1897.** Synthesis and characterization of 3D-oligothiophenes. **p. choong**, S. Valiyaveettil*
- 1898.** Long-lived and bright excimer emission of 9,10-bis(thienylethynyl)anthracene macrocyclic dimer. **H. Osaki**, C. Chou, M. Taki, Y. Sato, S. Saito, F. Aiko, T. Higashiyama, S. Yamaguchi*
- 1899.** Study toward living polymerization of aryne. **Y. Okada**, Y. Mizukoshi, K. Mikami*, M. Uchiyama*
- 1900.** Structural and electronic control of metal complexes by the use of π -systems. **A. Konishi**, R. Yasunaga, M. Yasuda*
- 1901.** Controlling of ICT fluorescence intensity of phenyldisilane with aza-crown ether. **D. Masuno**, Y. Inagaki, W. Setaka*
- 1902.** Oriented alignment and dichroism of a *p*-benzoquinone according to macrocage structure in crystal. **K. Sato**, Y. Inagaki, K. Yamaguchi, W. Setaka*
- 1903.** Graphite functionalization using electrochemically generated aryl radicals featuring various substituents. **B.D. Lindner**, T. Ishikawa, K. Tahara, J. Greenwood, T. Phan, S. De Feyter, Y. Tobe
- 1904.** Series of heterofluorenes containing four-coordinated group 13 elements. **T. Matsumoto**, K. Tanaka, K. Tanaka, Y. Chujo*
- 1905.** Molecular design of *cis* indigo and *cis* Nindigo. **H. Hong**, E.C. Nicholls-Alison, R. Hicks*
- 1906.** Two-photon excited NIR emissive dye with ESIP behavior. **N. Suzuki**, F. Aiko, M. Taki, K. Kamada, S. Yamaguchi*
- 1907.** Synthesis and properties of a doubly *N*-confused porphyrinoid with pyrrole[3,4-*f*]isoindole skeleton. **S. Hiraoka***, H. Uno, M. Takase, S. Mori, T. Okujima
- 1908.** Construction of hydrogen atom sandwich structure toward the reversible and effective proton and electron exchanging. **M. Teraoka**, Y. Hirao, T. Nishiuchi, T. Kubo
- 1909.** Photochemical and electrochemical properties of anthranol-acridine dyad. **Y. Hirao***, K. Hosoi, T. Nishiuchi, T. Kubo
- 1910.** Synthesis and photophysical properties of a pyrene-bridged molecular gyrotrop. **H. Shionari**, Y. Inagaki, K. Yamaguchi, W. Setaka*
- 1911.** Synthesis of condensed polycyclic compounds based on an acenaphthylene unit. **J. Nishida***, T. Kawase
- 1912.** Nonlinear absorption of polycyclic aromatic hydrocarbons with open-shell singlet character. **K. Kamada***
- 1913.** Material design for mechanochromic luminescence: 1,3,6,8-tetra[trialkylsilyl-ethynyl]pyrenes. **A. Orta***, T. Nishida, F. Xu, K. Shinohara, I. Kasuga, J. Otera
- 1914.** Synthesis and anti-aromaticity of 16 π anthracene-fused porphyrins. **R. Kuramasu**, S. Sugawara, Y. Yamamoto, S. Hiramatsu
- 1915.** Synthesis of distorted compounds by oxidation of aminophenanthrene derivatives. **H. Yokoi***, S. Hiroto, H. Shinokubo
- 1916.** Synthesis, structure, and optical properties of substituted tetracenes. **C. Kitamura***, G. Ohe, A. Takenaka, T. Kawase, T. Kobayashi, H. Naito
- 1917.** Rhodium-catalyzed enantioselective synthesis of benzopicene-based [9]helicene derivatives. **K. Murayama**, K. Tanaka*
- 1918.** Molecular design and some properties of stimuli-responsive brush-shaped π -conjugated polymers. **T. Ishikawa**, J. MOTOGANI, M. MINODA*
- 1919.** Theoretical study on the relationship between the open-shell singlet nature and the second hyperpolarizabilities of corannulene derivatives with two phenoxyl radical moieties. **Y. Minamida**, K. Fukuda, K. Yoneda, M. NAKANO
- 1920.** Generation and characterization of monoanion and dianion of a tetracyclo-penta[def,jkl,pqr,vwx]tetraphenylen derivative. **H. Miyoshi**, T. Kubo, Y. Tobe*
- 1921.** Significant enhancement of two-photon absorption probabilities by a substituent on the building block diphenylacetylene. **T. Isono***, S. Kinoshita, R. Takeuchi, T. Suzuki
- 1922.** Synthesis of multisubstituted dibenzophosphole oxides by intermolecular [2+2+2] cycloaddition. **T. Sato**, Y. Tahara, T. Shibata*
- 1923.** Synthesis and photophysical properties of pyrene-based blue light-emitting monomers. **T. Yamato***, X. Feng, H. Tomiyasu
- 1924.** Synthesis and unique optical properties of thiophene-BODIPY oligomers. **M. Saikawa**, S. Saino, M. Yamamura, T. Nabeshima
- 1925.** Synthesis of dihydroacridine derivatives with two pyridyl groups and their photophysical properties. **N. Maeda***, R. Suzuki, Y. Miura, N. Yoshioka
- 1926.** Chemical modification to 3-*tert*-butyl-1,5-diphenyl-6-oxoverdazyl radical by using Suzuki-Miyaura cross coupling reaction; crystal structure, optical and magnetic properties. **Y. Miura***, S. Ooshima, N. Yoshioka
- 1927.** Synthesis of asymmetric dinaphtho[2,3-*b*:2',3'-f]thieno[3,2-*b*]thiophene (DNNT) derivatives. **S. Lee**, H. Lee*
- 1928.** Synthesis of bis(anthroxyl) diradicals with proton coupled electron transfer activity. **I. Hattori**, Y. Hirao*, T. Nishiuchi, T. Kubo*
- 1929.** Synthesis, self-association, and anion recognition of conjugated macrocycles composed of carbazole and triazole moieties. **J. Satoshi**, S. Kato, Y. Nakamura*
- 1930.** Synthesis and photophysical properties of partially and fully overlapped [3,3](3,9)carbazolophane-alcohol derivatives. **T. Yashima**, K. Tani, K. Horii, K. Kubono, K. Sakakibara, Y. Tsuji
- 1931.** Synthesis and properties of [3,5](3,9)carbazolophane derivatives. **M. Asai***, K. Tani, K. Horii, H. Takemura, K. Sakakibara, Y. Tsuji
- 1932.** Ni(II) and Fe(III) complexes with pyridine ligands: Synthesis and PCET reactivity. **N. Tachibana**, Y. Hirao*, T. Nishiuchi, T. Kubo*
- 1933.** Synthesis and property of anti-aromatic ring by using the strain energy of non-planar pi-conjugated system. **K. SHIMIZU**, T. Nishiuchi, Y. Hirao, T. Kubo
- 1934.** Synthesis and properties of tetracene derivatives having diester groups on one terminal benzene ring. **M. Tsumura***, M. Takehara, Y. Inoue, C. Kitamura, T. Kawase, T. Kobayashi, H. Naito
- 1935.** Synthesis and quantum chemical calculations of sigmalene. **K. Sahara**, T. Nishiuchi, Y. Hirao, T. Kubo*
- 1936.** Synthesis and photophysical properties of carbazole chromophore containing Schiff bases and azo compounds. **K. Horii***, K. Tani
- 1937.** Synthesis and properties of anthracene-based cyclic Pi-cluster. **T. Nishiuchi***, Y. Hirao, T. Kubo
- 1938.** Lateral π -extensions of bisanthene toward a synthesis of oligoperfenes. **R. Ohkita***, T. Nishiuchi, Y. Hirao, T. Kubo
- 1939.** Synthesis and physical properties of oxygenated cycloparaphenelenes. **H. Onishi**, E. Kayahara, S. Yamago
- 1940.** Design and synthesis of solution processable, narrow band gap, near-IR absorbing small molecules. **A. Payne**, G. Welch*
- 1941.** Computational π -figuration of thiophene oligomers. **M. Sugimoto***
- 1942.** Synthesis, structures, and properties of biphenophinines tethered by aromatic system. **N. Nagahora**, H. Tokumaru, I. Takemoto, K. Shioji, K. Okuma
- 1943.** Synthesis of novel hydrogen-bonded charge-transfer complexes aimed at formation of PET state. **S. Seo**, Y. Hirao*, T. Nishiuchi, T. Kubo*
- 1944.** Construction of 3D architectures using alkyne metathesis. **S. Lee***, A. Yang, T. Moneyepenny, J.S. Moore
- 1945.** Synthesis and properties of binuclear paddlewheel-type complexes with azulene ligand. **R. Kawano**, T. Tsuchiya, S. Noro, Y. Mazaki

* Principle Author

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- 1946.** Synthesis and properties of viologen derivatives extended with azulene. **Y. Sano**, T. Tsuchiya, M. Hasegawa, Y. Mazaki
- 1947.** Facile synthesis for cyclic oligothiophene macrocycles by sulfides. **Y. Honda***, R. Inoue, M. Hasegawa, Y. Mazaki
- 1948.** Electron deficient tetrabenzo-fused pyracylene and conversions into curved and planar π -systems with distinct emission behaviors. **L. Chao***, M. Murata, Y. Sugano, A. Wakamiya, Y. Murata
- 1949.** Synthesis and optical properties of donor-acceptor molecules with aza[7]helicenes. **K. TAKASE**, K. Nakano*
- 1950.** Synthesis, properties, and OFET characteristics of π -conjugated systems having tetralozopyridine. **S. Tamai**, K. Hagiya, Y. Ie, Y. Asa
- 1951.** Synthesis of 9-aza-10-boraanthracene bearing transformable boron-chlorine bond synthesis of 9-aza-10-boraanthracene bearing transformable boron-chlorine bonds. **K. Suzuki***, K. Hayashi, S. Nema, M. Yamashita
- 1952.** Intramolecular carboannulation of 2-(arylethynyl)benzyl halide to indene derivatives: Toward a facile synthesis of s-indacene. **K. Fuji***, T. Nishizuchi, Y. Hirao, T. Kubo
- 1953.** Functionalization of the stable P-heterocyclic open-shell unit by the direct arylation. **Y. Ueta**, K. Mikami, S. Ito*
- 1954.** Synthesis and properties of anthracene bisimides incorporating triphenylamine donor units. **T. Iwanaga**, M. Ogawa, S. Toyota
- 1955.** Programmable arrangement of a metalloc-phthalocyanine and a metallo-porphyrin inside triply-stacked arrays. **N. Miura**, Y. Yamada, K. Tanaka*
- 1956.** Construction and properties of azulene templated binuclear metal complexes. **I. Kashiwagi**, T. Tsuchiya, Y. Mazaki
- 1957.** Design and synthesis of n-type donor-acceptor small molecules for use in organic solar cells. **A.D. Hendsbee**, A. Namespetra, E. Kitching, J. Sun, G. Welch*, I.G. Hill*
- 1958.** Synthesis of higher homologues of fused donors containing vinylogous TTF units and application to organic rechargeable batteries. K. Kawamoto, K. Hosoi, M. Kato, M. Yao, Y. Misaki*
- 1959.** Synthesis and properties of a cyclophane-type redox-responsive host containing two tetraphthalvalene units. **A. Ohta***, T. Kagami
- Hawaii Convention Center
Halls I, II, III
- Anion Receptors (#31)**
- Organized by: B. Hay, F. Pfeffer, B. Wu, C. Jia, R. Custelcean
- Poster Session**
19:00 – 21:00
- 1960.** Fluorescence probes for the detection of reactive oxygen species (ROS) and cyanide. **M. Atar**, A.G. Griesbeck*
- 1961.** Synthetic chloride transporters activated by enzymatic hydrolysis. **Y. Choi**, K. Jeong
- 1962.** Family of anionic LMOGs based on a phenylalanine-functionalised norbornene. **J.R. Engstrom***, F.M. Pfeffer
- 1963.** Indolocarbazole-pyridine foldamers: Helical folding and chloride transport ability. **H. Jeon**, K. Jeong
- 1964.** Selective colorimetric chemosensor with an electron-withdrawing group for multi-analytes CN^- and F^- . **T. Jo**, Y. Choi, S. Lee, J. Jung, H. Jang, J. Yun, K. Bok, C. Kim*
- 1965.** Highly selective fluorescent probe for detection of iodide ions. M. An, C. Lim, H. Seo, H. Kim*
- 1966.** Helical bias of indolocarbazole/pyridine oligomers with chiral segments. **J. Kim**, K. Jeong
- 1967.** Anion binding by ureido-substituted calixarenes. **O. Kundrat***, P. Curinova
- 1968.** Rational design, synthesis of reaction-based cyanide chemosensor in aqueous solution. **J. Li***, W. Dong
- 1969.** Design and synthesis of intramolecular charge transfer based fluorescent anion sensors. **S.M. Schutz**, J.B. Anderson, R.S. Muthyalu
- 1970.** Anion recognition properties of macrocyclic bisurea derivative based on 2,2'-binaphthalene. **A. Satake***, S. Kondo
- 1971.** Synthesis and evaluation of anion receptors having halogen bond donors. **S. Shibuya***, S. Kondo
- 1972.** Novel 1,8-naphthalimide-based anion sensor with an open space for an anion. **S. Nishino**, S. Ifuku, M. Morimoto, H. Saimoto, H. Izawa*
- 1973.** Anion recognition using fused [n]polynorbornane hosts and solid state examination of the host:guest complexes. **R. Robson**, F.M. Pfeffer*, L. O'Dell, J. Hook, R. Rawal
- 1974.** Fluorimetric detection of (chiral) anions by new urea-phenalimide dyads. **M. Vollmer**, S. Hanft, A.G. Griesbeck*
- 1975.** Can anion receptors control cation-exchange selectivity? **N.J. Williams**, C.O. Reynolds, L.W. Gill, R. Custelcean, B.A. Moyer
- 1976.** Strong binding affinity of triazole-bearing zinc porphyrin for anions by C-H hydrogen bonds. **D. Yim**, W. Jang*, C. Lee
- Hawaii Convention Center
Halls I, II, III
- Natural Product-based Drug Discovery (#66)**
- Organized by: B. Baker, R. Kerr, Y. Qin, D. Uemura, B. Littlefield
- Poster Session**
19:00 – 21:00
- 1977.** Synthesis and structure activity relationship study of Intervenolin and NBR16716 B, modulators of tumor-stroma interaction of natural origin. **H. Abe***, C. Sakashita, M. Kawada, J. Yoshida, H. Inoue, S. Ohba, T. Masuda, A. Nomoto, T. Watanabe, M. Shibasaki
- 1978.** Isolation of a pigment from a metagenomic library derived from the marine sponge *Halichondria okadai*. **T. Abe***, K. Miyamoto, Y. Sakakibara, T. Naito, D. Uemura
- 1979.** From genes to new molecules: Expression of silent fungal gene clusters in *Fusarium graminearum*. **D. Adressa***, L. Connolly, M. Freitag, S. Loesgen
- 1980.** Metabolomics approach to study the effect of *Andrographis paniculata* in improving chemotherapy treatment in colon cancer. **S. Ahmadi**, K. Shaari*, J. Stanlas
- 1981.** Search for amyloid β aggregation inhibitors from *Inonotus obliquus*. **Y. Aihara***, A. Kawaguchi, M. Takase, H. Shigemori
- 1982.** Alpha-glucosidase inhibitory activity and chemical analysis of the medicinal halophyte *Tamarix gallica*. **A. Ben Hmidene***, C. Abdelly, H. Isoda, H. Shigemori
- 1983.** Chemical investigation on the secondary metabolites of the aeolid nudibranch *Phyllodesmium lizardensis*. **A.S. Dewi***, K. Cheney, J.T. Blanchfield, M.J. Garson
- 1984.** GC-MS analysis of the β -N-acetylglucosaminidase inhibitor pochonicine and its analogs produced by a fungal strain. **K. Emoto**, Y. Mushake, A. Tsuchida, T. Okuda, H. Kanzaki, T. Nitoda*
- 1985.** Potential antidiabetic complications of isolated compounds from Indonesian traditional medicines. **S. Fatmawati***, W.D. Fitriana, M.D. Hidayati, F. Arianto, T. Ersam, K. Shimizu
- 1986.** Synthesis of biotin-introduced probe and analysis of target biomolecules of bisbromoamidine. **S. Fujikura**, O. Ohno, K. Suenaga
- 1987.** Chemopreventive activity of trichothecenes from *Trichothecium roseum* and their derivatives. **M. Fujiwara**, K. Shimoura, Y. Fukuda, M. Yamashita, A. Iida*
- 1988.** Proteasome inhibitors based on the natural product TMC-95. **M.G. Gotz**, D.L. Wilson, D. Krappmann, I. Meininger
- 1989.** Toward the total synthesis of (+)-neopeltolide: An oxa-conjugate route to the disubstituted 2,6-cis-tetrahydropyran ring system. **T.P. Hari***, B.I. Wilke, C.N. Boddy
- 1990.** Side-chain analogs of TAN-2483B as kinase inhibitors. **J.E. Harvey***
- 1991.** Search for bioactive substances from discomycete. **M. Haneda***, S. Seiki, T. Hosoya, H. Shigemori
- 1992.** Anti-oxidative constituents of the Brazilian traditional medicine, *Tabebuia avellaneda*. **R. Hidaka**, Y. Fukuda, M. Yamashita, A. Iida*
- 1993.** Use of principal component analysis Of ^1H - ^{15}N NMR spectra of amyloid- β (1-42) peptide for characterization of fibril formation inhibitors. **H. Hiroaki***, N. Iwaya, M. Matsuzaki, Y. Shigemitsu, N. Goda, Y. Abe, M. Hoshi, A. Narita
- 1994.** Stereocontrolled total synthesis of a stereoisomer of laurenifidin: Prediction of the stereochemistry of the natural product. **Y. Hori**, T. Yokoi, T. Inoue, T. Saka, A. Masuyama, S. Kobayashi
- 1995.** Synthesis and radical scavenging activity of C-methylated quercetin analog. **K. Imai**, I. Nakanishi, Y. Ohba, K. Matsumoto, K. Fukuhara*
- 1996.** Anti-allergic compounds from herbal medicines using newly developed assay method for stress-enhanced allergy. **K. Ishiguro***, H. Oku
- 1997.** Search of the excitatory substances to primary sensory neurons from natural resources using Ca^{2+} imaging method. **E. Iwaoka***, S. Yoshiyama, M. Nakaguchi, S. Fujigaki, Y. Dai, S. Aoki
- 1998.** Kurahyne, a novel ER stress-inducer isolated from marine cyanobacterial assemblages of *Lyngbya* sp. **A. Iwasaki**, O. Ohno, S. Sumimoto, K. Suenaga
- 1999.** Versicolamide B and 6-epi-stepachidin A isolated from *Aspergillus amoenum*: Biogenic implications. **H. Kato**, D. Sherman, R. Williams, S. Tsukamoto*
- 2000.** Synthesis and aldose reductase inhibitor activity of botryllazine B analogs having bicyclic heterocycles on the C6 position: A structure-activity relationship study. **R. Saito**, **A. Katoh**, K. Hitotsumatsu, K. Sasaki, T. Komatsu
- 2001.** Isolation and structure analysis of novel 9,11-seco-steroids from the sea hare *Aplysia kurodai*. **A. Kawamura**, M. Kitai, H. Kigoshi
- 2002.** Efforts towards the total synthesis of aziprasidic-3. D. Adu-Ampratwum, A. Okumu, **N. Kenton**, C. Forsyth*
- 2003.** Total synthesis and biological activity of sarcophytoloidi H. **T. Kikuchi**, H. Takamura, I. Kadota
- 2004.** Synthesis of aminocyclopentol analogs via stereoselective amination of cyclic polybenzyl ether with chlorosulfonyl. **Y. Kim***, J. JUNG, Y. Jung
- 2005.** Convergent synthesis of the HIJKL ring segment of ciguatoxin CTX3C. **T. Kimoto**, S. Hara, H. Takamura, I. Kadota*
- 2006.** Synthesis of O-methylated flavonoids and the studies on physiological functions of flavonoids. **Y. Kimura**, T. Kondo, K. Yoshida*
- 2007.** Stimulating a transcription in *Penicillium* sp. FKI-2140 activates a silent biosynthetic pathway to produce novel natural product. **S. Kishimoto**, M. Shimizu, N. Ishikawa, H. Noguchi, K. Watanabe
- 2008.** Total synthesis of (-)-leptistone. **Y. Kitabayashi**, S. Yokoshima, T. Fukuyama*
- 2009.** Studies on the search for bioactive substances from marine organisms. **S. Kobayashi**, Y. Kawazoe, D. Uemura*
- 2010.** Hydrolysis of a baker's yeast reduction product of oleuropein aglycon from olive leaf extracts. **M. Koga**, A. Takatsu, M. Jyo, K. Kikuchi, T. Nitoda, H. Kanzaki*
- 2011.** Bioactivity-guided isolation and structure elucidation of an anti-amyloid substance from *Psychotria stenorachya*. **A.V. Krivoshein***, A. Shottke
- 2012.** Neurotrophic compounds from Indonesian ginger bangle, *Zingiber purpureum*. **M. Kubo***, M. Nakai, K. Harada, N. Matsui, M. Akagi, M. Suenaga, Y. Matsunaga, Y. Fukuyama
- 2013.** Synthetic study on tomuruline. **C. Kudo**, O. Ohno, K. Same, K. Suenaga
- 2014.** Mutasyntesis of macrolactam antibiotics. **F. Kudo***, T. Eguchi
- 2015.** Isolation and structure of a novel and potent cytotoxic peptides from the marine cyanobacterium *Symploca* sp. **T. Kudo**, K. Sueyoshi, K. Fukumoto, S. Sumimoto, S. Suda, T. Teruya*
- 2016.** Development of curcumin-inspired hybrid molecules for the treatment of Alzheimer's disease. **A.A. Kulkarni***, E. Nwulia, S. Nekhai
- 2017.** Syntesis and inhibitory activity of as-cofurane derivatives against trypanosome alternative oxidase. **I. Kumamoto**, H. Saimoto*, H. Izawa, S. Ifuku, M. Morimoto, K. Kita*, D.K. Inaoka, M. Yamamoto
- 2018.** Synthetic study of a marine macrolide koshiklide and determination of absolute configuration. **K. Kunifuda***, A. Iwasaki, K. Suenaga
- 2019.** Isolation and structure elucidation of bioactive compounds from *Sanda cape*. **M. Kuramoto***, M. Sakamoto, Y. kurokawa, S. Mori, h. uno
- 2020.** Production of chemopreventive furanophenothiophenones by callus cultures of the Brazilian medicinal plant, *Tabebuia avellaneda*. **S. Kusakabe**, Y. Fukuda, M. Yamashita, A. Iida*
- 2021.** Antiplatelet effect of indothiazinone. **S. Kwon**, M. Jeong, M. Ryu, J. Jung
- 2022.** Synthesis and biological evaluation of antiangiogenen homoisoflavonane, cremastranone, and its analogs. **B. Lee**, X. Fei, H.D. Basavarajappa, D. Shin, T.W. Corson*, S. Seo*
- 2023.** Novel benzotates from traditional Chinese medicine prevent memory deficits. **J. Li***, L. Gao, L. Xiang
- 2024.** Parishin, an anti-aging phenolic glucoside from *Gastrodia elata*. **Y. Lin**, Y. Weng, L. Xiang, J. Qi*
- 2025.** Wewakazole B, a new cyclic dodecapeptide from the Red Sea cyanobacterium *Moorea producens*. **J.V. Lopez**, S.S. Al-Lihabi, W.M. Alarif, A. Abdel-latif, K. Washio, M. MORIKAWA, T. Okino*
- 2026.** Saccharothriolides A-C, novel phenyl-substituted 10-membered macrolides from a rare actinomycete *saccharothrix* sp. **S. Lu**, S. Nishimura, G. Hirai, M. Ito, T. Kawahara, M. Izumikawa, M. Sodeoka, K. Shin-ya, T. Tsuchiwa, H. Kakeya*
- 2027.** Discovery of biologically active natural products from Philippine Annonaceae plants and their associated fungi. **A.G. Macabeo***, P. RUBIO, A. LETADA, R. MENDOZA, I. MALALUAN, I. FLORES, J. ABANTO, F. MARTINEZ, A. LOPEZ, F. TUDLA, E. PARAGAS, M. KNORN, P. KOHLS, C. FADERL, H. DAHSE, G.D. ALEJANDRO, S. FRANZBLAU
- 2028.** Phytochemical and pharmacological evaluation of *Sida rhombifolia*. **S. Mah***, S. Teh, G.C. Ee
- 2029.** Chemical approaches to selective elimination of human pluripotent stem cells. **D. Mao**, T. Kuo, E. Kawase, S. Sato, M. Uesugi*
- 2030.** New coumarin analogs and their antimicrobial activity. **A. McElrea**, A. Ata*

*** Principle Author**

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- 2031.** Phytochemical analysis of *Rhamnus caroliniana*. **A. Mekala**, W.N. Setzer
- 2032.** Study on the enzymatic construction of polycyclopropane skeleton in jawsamycin biosynthesis. **A. Minami**, T. Hiratsuka, H. Oikawa*
- 2033.** New naphthoquinone and monoterpenoid from *Plumbago zeylanica*. **T. Mitsui**, C. Miyachi, Y. Ishimura, K. Oda, K. Hayashi, A. Kuboki, S. Ohira, N. Matsura, I. Munekazu, H. Nozaki*
- 2034.** Synthesis and biological evaluation of hydroxamate amides as HDAC inhibitors. **H. Mok**, K. BAEK, H. SON, Y. Jung
- 2035.** Synthetic study of enigmazole A. **Y. Murai**, T. Kishi, Y. Fujisawa, H. Takamura, I. Kadota*
- 2036.** Synthesis and biological activity of citridone A and its analogs. K. Shimoyama, T. Fukuda, H. Tomoda, **T. Nagamitsu***
- 2037.** Synthesis of novel pentacyclic derivatives with propellane skeleton and their structure-activity relationships. **R. Nakajima***, N. Yamamoto, S. Hirayama, T. Iwai, T. Nemoto, H. Fujii, H. Nagase
- 2038.** Solvent effect on the radical-scavenging mechanism of ascorbic acid and its derivatives. **I. Nakaniishi***, K. Ohkubo, K. Inami, S. Nomura, K. Fukuhara, K. Matsumoto, T. Ozawa, S. Fukuzumi, M. Mochizuki
- 2039.** Isolation of new metabolites from a microbial metabolites fraction library by NPPlot screening. **T. Nogawa**, A. Okano, J. Jang, T. Shimizu, S. Takahashi, H. OSADA*
- 2040.** Novel screening approach for drug discovery from virtual mirror-image library of natural products. **T. Noguchi**, S. Oishi, K. Honda, Y. Kondoh, T. Saito, H. Ohno, H. Osada, N. Fujii
- 2041.** *Diospyros macrocarpa*: An endemic plant of New Caledonia with biological activities. C. Thieury, R. Le Guével, C. Anthaumea, G. Herbette, V. Monnier, N. Lebouvier, E. Hnawia, T. Guillaudeau, M. Nour
- 2042.** Janadolide, an apoptosis-inducing cyclic lipopeptide possessing a *t*-Bu group from the marine cyanobacterium *Oceania lorea*. **H. OGAWA**, A. Iwasaki, S. Sumimoto, O. Ohno, K. Suenaga
- 2043.** Highly efficient synthesis of unnatural spinasterol glucose analogs and repressed expression of the skin inflammatory mediators in human keratinocytes. h. kim, t. lee, T. Kim, **H. OH**
- 2044.** Biosynthesis of a cancer-inducing compound in *Escherichia coli*. **M. Ohashi**, Y. Sasa, N. Ishikawa, H. Noguchi, K. Watanabe*
- 2045.** Production of chemopreventive naphthoquinones by callus cultures of *Catalpa bungei*. **M. Ohmiya**, Y. Fukuda, M. Yamashita, A. Iida*
- 2046.** Structure-activity relationship study and total synthesis of pyripyropine A as a potent ACAT2-selective inhibitor. **M. Ohtawa**, T. Ohshiro, S. Omura, H. Tomoda, T. Nagamitsu*
- 2047.** Total synthesis of mycalolide B, an actin-depolymerizing marine macrolide. **H. Oka**, M. Kita, H. Kigoshi
- 2048.** Total synthesis of kurahynes: A new acetylene-containing lipopeptide from marine cyanobacterial assemblage. **S. Okamoto**, A. Iwasaki, O. Ohno, K. Suenaga
- 2049.** Highly efficient synthesis of β -Lapachone and its derivatives. h. kim, H. Lee, T. Han, G. Lee, B. Kim, **s. park**
- 2050.** Total synthesis of (+)-hyacinthacine A2 via regioselective and diastereoselective amination with chlorosulfonyl isocyanate. **S. Park***, I. JIN, M. Choi, Y. Jung
- 2051.** Total synthesis of conduramine D-1 via a highly regioselective and diastereoselective allylic amination using chlorosulfonyl isocyanate. **S. Park***, Y. Jung
- 2052.** Chemical synthesis and preliminary PK/PD studies of PBRM, a novel inhibitor of 17 β -hydroxysteroid dehydrogenase type 1. **D. Poirier**, R. Maltais, J. Roy, A. Trottier
- 2053.** Isolation of antileishmanial compound from *Sassafra s albidum*. **D. Pulavarthi**, **K.M. Steinberg**, L. Monzote, W.N. Setzer
- 2054.** Synthesis of indothiazinone via direct 3-acylation. **M. Ryu**, S. Kwon, M. Jeong, J. Jung
- 2055.** Design and synthesis of a molecular shuttle to transport cargo into Gram-negative bacteria. **J.A. Saboury**, C. Bezjian, A. Davidian, A. Avanes, B. Ulloa, M. Pinto, C. Gutierrez*
- 2056.** Isolation, purification, and structure identification of cytotoxic compound(s) from *Piper nigrum* black peppercorns. **V.S. Santiago***, I.M. Villaseñor
- 2057.** Synthesis of biselyngbyasides. **E. Sato**, Y. Tanabe, N. Nakajima, A. Ohkubo, K. Suenaga*
- 2058.** Total- and semi-synthetic approaches towards new analogs of colchicine. **W. Schlundt***, H. Schmalz
- 2059.** Secondary metabolites from *Achyranthes aspera* (chirchitta). **R. seharawat**
- 2060.** Induction of hepatocyte growth factor production in human dermal fibroblasts by caffeic acid derivatives. **H. Shigenori***, M. Kurisu, R. Nakasone, Y. Miyamae, D. Matsuma, H. Kanatani, S. Yano
- 2061.** Kuji amber extract has anti-allergic effect and a spirolactone compound is also involved in the activity. **E. Shimizu***, M. Kobayashi, H. Koshino, T. Uchida, Y. Okawa, H. Shinden, S. Uesugi, K. Kimura
- 2062.** New modified total synthesis and modular derivatization of indolactam. **J.E. Stein**, H. Schmalz*
- 2063.** Synthetic approach toward the natural product, suberadamine A. **N.T. Stessman***, K. Chan, C. Cerpas, B. Gill, E. Grollé, B. Ishaya, C. Stessman
- 2064.** Odoamide, a novel cyclodepsipeptide from marine cyanobacterium *Symploca* sp. **K. Sueyoshi**, M. Kaneda, S. Oishi, N. Fujii, S. Sumimoto, S. Suda, T. Teruya*
- 2065.** Structure of novel linear lipopeptides which contained unique fatty acid, isolated from a marine cyanobacterium. **S. Sumimoto***, A. Iwasaki, O. Ohno, T. Teruya, T. Inuzuka, K. Suenaga
- 2066.** Study on the search for natural products from dinoflagellate which inhibit protein kinase GSK-3 β . **T. Suzuki**, J. Yabe, Y. Kawazoe, D. Uemura*
- 2067.** Structure determination of proanthocyanidins by combination of H/D exchange and MS/MS. **H. Takahashi**, K. Hamaoka, T. Kusumi, K. Ohmori, K. Suzuki
- 2068.** Synthetic study on the antitumor cyclopeptide metabolite, verucopeptin. **N. Takahashi**, H. Hayashi, H. Kakeya*
- 2069.** Comparative studies on the hydroperoxide compounds and the endoperoxide compound isolated from *Calcaria delphinifolia*. **Y. Takahashi***, S. Uesugi, Y. Takano, N. Usukhbayar, E. Tsuchiya, H. Koshino, K. Kimura
- 2070.** Insecticidal and growth inhibitory activities of metabolites of fungal strains producing β -N-acetylglucosaminidase inhibitors against larvae of sheep blowfly. **E. Takatsuji**, T. Okuda, H. Kanzaki, T. Nitoda*
- 2071.** Total syntheses of the nonpeptide Bradykinin B1 receptor antagonist velutinol A and its derivatives, the seco-pregnanes with cage-like moiety. M. Tamai*, N. Isaka, T. Kitazawa, M. Ishiguro*
- 2072.** Promising drug candidates from natural sources: Amphidinolide H, eudistomin C, and biyouyanagin A. **N. Tanaka***, J. Kobayashi
- 2073.** Synthetic study of (-)-dactyliolide. **T. Tanaka**, Y. Murai, H. Takamura, I. Kadota*
- 2074.** Neuroprotective effect of biflavones isolated from leaves of *Sciadopitys verticillata*. **Y. Tanaka**, Y. Hirata, D. libata, S. Kitayama, M. Tamano, Y. Yoshimoto, N. Fukata, T. Sumiyoshi, Y. Nagaoka*
- 2075.** Structure modification and structure-activity relationships of bioactive sporogen AO-1. **C. Tansakul***, V. Rukachaisirikul, C. Daengrot, N. Supantanapong, C. Tantisuwanno, S. Phongpaichit, J. Sakayaroj
- 2076.** Synthesis of α,α -disubstituted hydantoins through chemoselective derivatization of natural product extracts. **K. Tomohara***, A. Kato, I. Adachi
- 2077.** Novel cytotoxic diterpenes from a marine myxobacterium, *Enhygromyxia* sp. **T. Tomura**, R. Fudou, T. Iizuka, M. Ojika*
- 2078.** Overcoming natural product purification Co-eluting peaks with recycling prep HPLC. **K. Tseng**, I. Hidet
- 2079.** Fungal simplifungin and valsafungin, new antifungal antibiotics targeting serine palmitoyltransferase. **R. Uchida**, H. Ishijima, M. Ohtawa, A. Kondo, K. Nagai, K. Nonaka, R. Masuma, S. Iwamoto, H. Onodera, T. Nagamitsu, H. Tomoda
- 2080.** Study on biological activities and molecular targets of alantopyrone A and pyrocidine A isolated from endophytic fungi. **S. Uesugi***, M. Muroi, Y. Kondoh, Y. Shiono, H. OSADA, K. Kimura
- 2081.** Design, synthesis, and biological evaluation of photosensitizers bearing a high water solubility. **Y. Urura**, T. Nonomura, M. Edatani, K. Onuma, F. Okada
- 2082.** New phenylethanoid glycosides from *Magnolia officinalis* fruits. **Y. Wang***, L. Ge, B. Ma, G. Zhou, W. Zhang, L. Chen, Z. Zhou
- 2083.** Novel physiological roles of mango seed oil using proteomic analysis of differentially expressed proteins. **s. Wu***, k. Matsumoto, s. TACHIBANA, t. INOUE, m. NOMURA
- 2084.** Studies towards the total synthesis of palanine type of *Lycopodium* alkaloids. **S. Xu***, Y. Gong, X. Wang, S. Zhang
- 2085.** Synthetic studies of biologically active mannosilated 3-acyltetrameric acids. **A. Yajima***, C. Ida, A. Kawajiri, R. Katsuta, T. Nukada
- 2086.** Structures and bioactivities of okeanamide and chlorookeanamide from marine cyanobacterium *Oceania* sp. **M. Yamada**, K. Sueyoshi, T. Yonezawa, B. Cha, J. Woo, S. Sumimoto, S. Suda, T. Teruya*
- 2087.** Elucidation of pyranonigrin biosynthetic pathway reveals mechanism of fused γ -pyrone, exo-methylene and spiral cyclobutane formation. **T. Yamamoto**, Y. Tsunematsu, H. Noguchi, K. Hotta, K. Watanabe*
- 2088.** Marine natural products with protein tyrosine phosphatase 1B inhibitory activity. **H. Yamazaki***, S. Kanno, O. Takahashi, R. Kirikoshi, D.B. Abdulj, K. Ukai, H. Rotinsulu, D.S. Wewengkang, D.A. Sumlat, R.E. Mangindaan, M. Namikoshi
- 2089.** Induced production of new epidithiodiketopiperazines by the Palauan marine-derived fungus *Trichoderma* sp. TPU199. **H. Yamazaki***, O. Takahashi, R. Kirikoshi, M. Namikoshi
- 2090.** Synthetic study of optically active valerenic acid analogs for development of sedative active compounds. **S. Yato**, Y. Izu, T. Shirai, H. Tsunagata, T. Kitayama
- 2091.** Effect of the Brazilian medicinal plant *Myrcia sphaerocarpa* on hyperglycemia and its active constituents. **M. Yoneda**, Y. Fukuda, M. Yamashita, A. Iida*
- 2092.** Synthetic studies on ecteinascidin 743. **E. Yoshida**, T. Toma, S. Yokoshima, T. Fukuyama*
- 2093.** Ethnomycology directed discovery: Expanding the chemistry of *p*-terphenyl natural products. **M. Zhang***, A.M. Beekman, R. Barrow
- Hawaii Convention Center
Halls I, II, III
- Molecular Containers (#99)**
- Organized by:** S. Mitsuhiiko, L. Isaacs, H. Yang
- Poster Session**
19:00 – 21:00
- 2094.** Gating of catalysis by self-assembled nanospheres with multiple endohedral binding sites. **Q. Wang**, J.N. Reek*
- 2095.** Metallo molecular containers with tetrakis(2,2'-bipyridyl)porphyrin ligands. **H. Ube**, T. Nakamura, R. Miyake, S. Watanuki, K. Endo, M. Shiro, M. Shionoya*
- 2096.** Construction of a transformable coordination capsule/tube with polycationic frameworks. **K. Yazaki**, Y. Sei, M. Akita, M. Yoshizawa*
- 2097.** Cationic ligands as building blocks for molecular containers: Guest binding through host-anion-guest interactions. **A. Peuronen***, A. Taponen, S. Forsblom, M. Lahtinen*
- 2098.** Dinuclear-Ag(I)-macrocycle: Recognition of ditopic aromatic molecules through multipoint Ag- π interactions. **K. OMOTO**, S. Tashiro, M. Kuritani, M. Shionoya*
- 2099.** Selective recognition of steroid hormones by using an M_2L_4 coordination capsule. **M. Yamashina**, M. Akita, M. Yoshizawa*
- 2100.** Synthesis of self-assembling biscavitanoids for molecular recognition and guest complexation. **M. Escamilla***, J.P. Buenafior, L. Tunstad
- 2101.** Polycromatic capsule capable of detecting natural fragrance compounds. **A. Suzuki**, Y. Sei, M. Akita, M. Yoshizawa*
- 2102.** Multiresponsive metal-organic lantern capsules in solution. **J.K. Klosterman**
- 2103.** Facile synthesis, structures, and guest binding properties of resorcinol-bridged cofacial porphyrin dimers. **N. Kuramochi**, K. YAMASHITA*, Q. PHAM, K. KATAOKA, K. SUGIURA
- 2104.** Enzymatic activity of CLE confined within M_{12-24} spherical complex. **Y.E. Fujii**, D. Fujita, M. Fujita*
- 2105.** Inclusion ability of cyclic porphyrin dimers directed toward preparation of π -conjugated molecular tube. **Y. Chiba**, J. Terao, T. Fujihara, Y. Tsuji*
- 2106.** Inverse electron demand Diels-Alder reactions for tuneable post-assembly modification. **B.S. Pilgrim**, D.A. Roberts, J.D. Cooper, J.R. Nitschke*
- 2107.** Shape-selective solid state host-guest complexation between pillar[5]arene and n -alkanes with gate opening pressure. **R. Sueto**, T. Ogoshi, T. Yamagishi
- 2108.** Synthesis and evaluation of new functional materials using hyperbranched polymer. **R. Sato**
- Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4
- Recent Trends in Organocatalysis (#122)**
- Organized by:** M. Terada, M. Shi, J. Antilla, K. Maruoka
Presiding: S. Takizawa, M. Terada
- 19:00 – 2109.** Synthetic study of biologically active piperidine alkaloids using asymmetric organocatalytic reactions. **H. Ishikawa***
- 19:20 – 2110.** Catalyst control of diastereoselectivity in chiral amine-catalyzed asymmetric conjugate additions of aldehydes. **T. Kano***, K. Maruoka*
- 19:40 – 2111.** Novel bifunctional phosphonium(or ammonium) salts based on amino acids: cooperative phase-transfer catalysis in asymmetric C-C bond forming reaction. **G. Zhao**

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- 20:00 – 2112.** Asymmetric catalysis of *P*-spiro chiral tetraaminophosphonium salts. **D. Uraguchi***
- 20:20 – 2113.** Enantioselective organocatalyzed formal [n+2] cycloaddition using alkenoates. **S. Takizawa***, H. Sasaki
- 20:40 – 2114.** Development of organocatalyst and its application toward the synthesis of bioactive natural product. **T. Yamada**, T. Hirose, S. Omura*, T. Sunazuka*

Hawaii Convention Center
Halls I, II, III

Organic Reactions in Aqueous Media (#131)

Organized by: S. Kobayashi, B. Lipshutz, C. Cai

Presiding: S. Kobayashi

Poster Session

19:00 – 21:00

- 2115.** Quantitative reaction monitoring of heterogeneous reactions in water by using DART-MS. **K. Masuda**, S. Kobayashi

- 2116.** Development of catalytic construction of hydrogen isotope chirality in deuterium oxide. **T. Kitanosono**, S. Kobayashi

- 2117.** Chiral copper(II) catalysts for enantioselective silyl conjugate additions in water. **T. Kitanosono**, C. Liu, L. Zhu, P. Xu, S. Kobayashi

- 2118.** Design of novel catalysts in water utilizing interaction between Lewis acid-surfactant-combined catalyst and single-walled carbon nanotube. **P. Xu**, T. Kitanosono, S. Kobayashi

- 2119.** Palladium(II)-catalyst mixed with surfactant for Michael reactions in water. **M. Miyo**, T. Kitanosono, S. Kobayashi

- 2120.** Development of asymmetric Mukaiyama aldol reactions without use of organic solvent. **L. Zhu**, T. Kitanosono, S. Kobayashi

- 2121.** Conversion of nitroalkanes into carboxylic acids via iodide catalysis. **P. Marce-Villa***, J. Lynch, J.M. Williams

- 2122.** Photocatalytic carbon-carbon bond forming reaction in aqueous media. **H. Miyabe**

- 2123.** Green protocol for the synthesis of vesicular acetylcholine transporter inhibitors and beta blockers. **J. Agarwal***

- 2124.** Synthesis of an amphiphilic *N*-heterocyclic carbene ligand applicable to the aqueous cross coupling reaction. **T. Yanagimoto***

- 2125.** Organic reactions in aqueous Triton X-100 (TX100) micelles. **G. Lu**

- 2126.** Hydrophobic effect in the reaction of amphiphilic thioesters with alkyl amines in water. **I. Otomo**, C. Kuroda

- 2127.** Asymmetric reduction in aqueous aggregates formed from a chiral surfactant. **Y. Ono**, Y. Takahashi, Y. Kondo*

- 2128.** Asymmetric aldol reaction of hydroxyacetone and dihydroxyacetone derivatives catalyzed by chiral Zn^{2+} complexes of aminoacyl 1,4,7,10-tetraazacyclododecane. **M. Yasuda**, S. Itoh, S. Aoki

- 2129.** Catalytic hydration of organonitriles catalyzed by O-donor ligated iridium complexes. **T. Oshiki***

- 2130.** Synthesis of *N*-heterocyclic carbine-based surfactants and their catalytic activities in aqueous solution. **T. Taira***, T. Yanagimoto, K. Sakai, H. Sakai, A. Endo, T. Imura

- 2131.** Design of nano-scale platform for Diels-Alder reaction in water using liposome. **F. Iwasaki**, K. Suga, Y. Okamoto, H. Umakoshi*

- 2132.** Green *a*-bromination of arylketones with $HBr-NaClO_2$ in water. **S. Ko**, J. Ban, Y. Jung, H. Rhee*

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Applications of C-H Functionalization (#169)

Organized by: P. Vachal, Z. Shi, C. Li, H. Davies, K. Itami, H. Lebel

- 19:00 – 2133.** New stage of chelation assisted functionalization of C-H bonds. **N. Chatani***

- 19:30 – 2134.** Directing group-free copper-catalyzed intermolecular arylation of simple primary and secondary benzylic sp^3 C–H bonds. **S. Zultanski**, S.S. Stahl*
- 19:50 – 2135.** Access to tetrahydroisoquinolines via intramolecular direct functionalization of alpha-cyclopoly amino acid-derivatives. **C.L. Ladd**, A.V. Belouin, A.B. Charette*
- 20:10 – 2136.** Development of novel iridium complexes for enantioselective atom transfer C–H functionalizations. **S.B. Blakey***
- 20:40 – 2137.** Transition metal-free direct functionalization of arene C–H bonds: Rapid synthesis of biaryls, aryl ketones as well as fused N- and O-heterocycles. **L. Kurti***

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 4

Strategies and Tactics for Complex Molecule Synthesis (#174)

Organized by: C. Forsyth, C. Lee, L. Barriault, J. Cha

Presiding: A.E. Mattson, M. Visco

19:00 introduction

- 19:00 – 2138.** Synthetic studies on the *Galbulimima* alkaloid GB17. **R. Thomson***

- 19:25 – 2139.** Catalytic enantioselective vinyllogous Pictet-Spengler reaction: Toward the total synthesis of the Kopsia alkaloids. **U.K. Tambar**

- 19:50 – 2140.** Efforts towards the total synthesis of bisbelyngbyolide a. **K. Nostadt**, M.E. Maier*

- 20:00 – 2141.** Progress toward the total synthesis of Ivorenolide A. **M. de Leseleuc**, E. Godin, S. Parisien-Collette, S. Collins*

- 20:10 – 2142.** Analog-oriented synthesis of bioactive natural products. **C. Vanderwal**

- 20:35 – 2143.** Catalytic enantioselective carbon–carbon bond formation reactions with diazo compounds. **D. Ryu***, B. Kang, S. Shin, S. Shim

Hawaii Convention Center
Halls I, II, III

New Organosulfur Chemistry (#436)

Organized by: E. Block, E. Juaristi, A. Schwan, X. Jiang, C. Lee

Presiding: R. Glass

Poster Session

19:00 – 21:00

- 2144.** Novel preparation of cyclic vinyl sulfones and alkylalkynyl sulfones. **A. Rodríguez Menéndez***

- 2145.** Stereoselective synthesis of chiral sulfilamines and sulfoximines. **H. Piras**, H. Lebel*

- 2146.** Reaction scheme for "pinking" of onion. M. Kato, T. Kamoi, S. Imai*

- 2147.** Access to thiacycles via Pd-catalyzed cascade cyclizations. T. Castanheira*, M. Donnard, J. Suffert, **M. Gulea***

- 2148.** Biobased thioethers as metal-absorbing ligands. R.E. Murray*, **G.B. Bantchev***, R.O. Dunn, K.L. Ascherl, K.M. Doll

- 2149.** Thiol-ene chemistry of vinylidemethyl-lactones in $CDCl_3$. **F. Azemar***, J. Pinaud, S. MONGE

- 2150.** Exceptionally simple chiral sulfur-based olefin ligands for broad-scope asymmetric catalysis. **M. Xu***

- 2151.** Copper-catalyzed aerobic oxidation of thiols for the synthesis of thiocarbonyl compounds. **H. Jang***

- 2152.** Stereoselective synthesis of *cis*- α,β -unsaturated sulfones and sulfonates using new Peterson reagents. **K. Ando***, M. Okumura, H. Sumida, T. Wada, K. Fujimoto

- 2153.** Ruthenium complex-controlled catalytic addition of organic disulfides to terminal alkynes. **K. Sawase***, Y. Kimura, A. Toshimitsu, T. Kondo

- 2154.** New insights into the electronic structures and electrochemical behavior of 2-benzothio- and 2-benzoselenopyrlyum tetrafluoroborates. **N. Nagahora**, I. Takemoto, M. Fujii, H. Tokumaru, K. Shioji, K. Okuma

- 2155.** Furocene-fused sulfur heterocycles. S. Banks, B. Maharjan, **J.P. Selegue***, S. Parkin

- 2156.** Synthesis of sodium sulfinites and their application in palladium(II) catalyzed addition reactions. **B. Skillinghaug**

- 2157.** Copper-catalyzed preparation of thiosulfonates using sodium sulfinites with thiols or disulfides. **N. Taniguchi***

- 2158.** Selective S-deacetylation: Practical syntheses of glycosylthiols and drug mercapto-analogs. P. Shu, J. Zeng, J. Tao, Y. Zhao, Q. Wan*

- 2159.** Tandem reactions leading from simple sulfones to complex bicycles and tricycles: Applications as enzyme inhibitors. **J.E. Wulff***, M.G. Brant

- 2160.** Thio-click and domino approaches to thioglycomimetics. **Z. Witczak***

Saturday Morning

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25)

Organized by: T. Kubo, Y. Tobe, M. Haley, G. Bodwell, K. Wong

Presiding: K. Wong

- 8:00 – 2161.** Insulated oligothiophene molecular wires and tripod anchors for molecular electronics. **Y. Aso***

- 8:40 – 2162.** Selenium and tellurium-containing organic electronic materials. **D.S. Seferos**

- 9:05 – 2163.** Thiophene-fused dehydroannulenes: An isolable, but reactive scaffold for polycyclic 2D π electron systems. **F. Aiko***

- 9:30 – 2164.** Contorted aromatics and polymers from cyclopenta-fused polycyclic aromatic hydrocarbons. **K.N. Plunkett**

- 9:45 – 2165.** Thiophene-containing macrocyclic arelenes: Synthesis and photophysical properties. **T. Shibata***, S. Kita, M. Fujimoto, Y. Suzuki, D. Yokoyama

- 10:00 – 2166.** Designing aromatic structures to help control molecular organization in thin-layer devices. **J. Wuest***, A. Heskia, S. Langis-Barrette, V. Lachapelle

- 10:40 – 2167.** 2D polymers as lattice templates for designer surfaces. **B.T. King**

- 11:05 – 2168.** From open-shell singlet diradicals to polyradicaloids. **J. Wu**

- 11:30 – 2169.** Copper-catalyzed efficient route to 2-halo-substituted imidazo[1,2-*a*]pyridines and its application in designed pi-electronic systems. **H. Jiang***, Y. Gao, W. Wu

- 11:45 – 2170.** Synthesis and characterization of 3,3'-5,5' doubly linked corrole dimers. **T. Tanaka**, S. Ooi, A. Osuka*

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Anion Receptors (#31)

Organized by: B. Hay, F. Pfeffer, B. Wu, C. Jia, R. Custelcean

Presiding: R. Custelcean, P. Gale

- 8:00 – 2171.** Power of the chelate and macrocyclic effects in anion coordination. **K. Bowman-James***, H. Telikepalli, P. Metola, V. Day

- 8:30 – 2172.** Hydrogen bond host for fluoride and (maybe) hydride. **J. Jackson**, T. Kakeshpour, P. Nandi

- 9:00 – 2173.** Ion pair-based molecular recognition of biological targets by supramolecular ligands. **C. Schmuck***

- 9:30 – 2174.** Pseudo-bicyclic guanidinium-based scaffold for binding anions in a symmetric planar conformation. **V. Bryantsev**, C.A. Seipp, N.J. Williams, R. Custelcean, B.A. Moyer

10:00 Break

- 10:15 – 2175.** Calixpyrroles as anion and ion pair receptors. **J.L. Sessler***

- 10:45 – 2176.** Peptidic receptors for selective anion recognition in aqueous solution. **K.A. Jolliffe***

- 11:15 – 2177.** Cooperativity and complexity in the binding of anions and cations to a tetrapotic ion-pairing host. **P. Thordarson***, E. Howe

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Natural Product-based Drug Discovery (#66)

Organized by: B. Baker, R. Kerr, Y. Qin, D. Uemura, B. Littlefield

Presiding: H. Kigoshi, D. Romo

- 8:00 – 2178.** Microtubule-stabilizing natural products: potential agents for neurodegenerative disease. **A.B. Smith**, III, V.M. Lee, J.Q. Trojanowski, K.R. Brunden, I. Paterson, C. Ballatore

- 8:35 – 2179.** Aplyronine A, an antitumor marine macrolide that promotes protein-protein interaction. **H. Kigoshi***

- 9:05 – 2180.** Bioactivity-guided retrosynthesis: "Upping the ante" for natural product-based drug target and lead discovery. **D. Romo***

- 9:40 – 2181.** Isolation and total synthesis of microbial natural products. **T. Sunazuka***, T. Hirose, S. Omura

- 10:00 – 2182.** Discovery of bioactive lead compounds from plants. **H. Zhang***

- 10:20 – 2183.** Formal total synthesis of sarain A. S. Yokoshima

- 10:40 – 2184.** Convergent approach to the synthesis of ciquatoxin CTX3C. **I. Kadota***

- 11:00 – 2185.** "Re-tooling" natural products for drug discovery. **C.L. Chai**

- 11:10 – 2186.** Discovery of novel orexin receptor agonists for controlling sleep/awake cycle. **T. Saitoh**, T. Nagahara, N. Kutsunura, Y. Irukayama, Y. Ogawa, H. Fujii, M. Yanagisawa, H. Nagase

- 11:20 – 2187.** Unified total synthesis and biological activity of sarcophytolides. **H. Takamura***, K. Iwamoto, E. Nakao, N. Harada, T. Kikuchi, O. Ohno, K. Suenaga, N. Endo, Y. Fukuda, I. Kadota

- 11:30 – 2188.** Construction of congested bridged bicyclic systems: Progress toward the first total synthesis of an anti-thrombotic natural product. S.L. Maki, E.J. St.Germain, K.P. Yadavalli, P. Maity, **S.D. Lepore***

Hilton Hawaiian Village
Halls I, II, III

Recent Trends in Organocatalysis (#122)

Organized by: M. Terada, M. Shi, J. Antilla, K. Maruoka

Poster Session

10:00 – 12:00

- 2189.** Stereoselective aldol reactions using organocatalysts having a 2,6-difluorophenyl group derived from (L)-valine. **Y. Tanimura, K. Ishimaru***

- 2190.** Phosphine oxide-catalyzed enantioselective cross-aldol reactions between ketones. **S. Kotani***, S. Aoki, M. Suguri, M. Ogasawara, M. Nakajima

* Principle Author

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- 2191.** Fluorogenic probes for chemical transformations: Turn-on aldol, Mannich, and Diels-Alder reaction sensors for evaluation of both enamine and iminium catalysts. **N. Mase***, T. Masuda, K. Sato, T. Narumi, N. Watanabe
- 2192.** Activation of boron compounds by chiral α -hydroxy carboxylic acid catalysts. **M. Sugiyra***, Y. Kuboyama, W. Ishikawa, M. Tokudomi, R. Kinoshita, M. Nakajima
- 2193.** Regio- and stereoselective conjugate addition of aldehydes to β -tosyl enones catalyzed by binaphthyl-modified chiral amine. **H. Maruyama**, H. Sugimoto, T. Kanou, K. Maruoka
- 2194.** Development of 1,4-addition reaction of 2-formylthioesters to vinylketones involving an all-carbon quaternary carbon atom construction. **T. Misaki***, T. Tatsumi, T. Sugimura
- 2195.** Enantioselective phase-transfer catalytic alkylation of (*E*)-4-bromobenzylidene-neamino *tert*-butyl malonates. **C. Park***, M. Ha, D. Kim, S. Hong, Y. Park, M. Kim, H. Park
- 2196.** Novel method for synthesis of cyclic ether using transition metal catalysts. **R. Nakaya**, H. Yokoyama, M. Miyazawa*
- 2197.** Chemoselective two-directional reaction induced by acidic zwitterions bearing highly stabilized carbion moiety. **H. Yanai**, Y. Sasaki, Y. Yamamoto, T. Matsumoto
- 2198.** Synthesis of novel quaternary ammonium salts derived from quinine and their application to asymmetric hydrolysis of amino acid esters. **Y. Furutachi***, Y. Hidani, T. ISHIDA, M. Tokunaga, A. Hamasaki
- 2199.** Theoretical study on enantioselective alkylation by binaphthyl chiral phase-transfer catalysts: A DFT-based conformational analysis. **T. Kamachi**, K. Yoshizawa
- 2200.** Final-stage site-selective acylation for the total syntheses of multifidisides A-C by organocatalysis. **Y. Ueda**, T. Furuta, T. Kawabata*
- 2201.** Oxy-alkyl cation mediated asymmetric nucleophilic substitution of α -tosyloxy cyclopentanones. **C. Liu***, E.Z. Oblak, M. Vanderwal, D. Almstead
- 2202.** Straightforward synthesis of 1,2-di-cyanoalkanes from nitroalkenes and silyl cyanide mediated by tetrabutylammonium fluoride. **T. Nagata**, K. Kiyokawa, S. Minakata*
- 2203.** Phase-transfer catalyzed asymmetric synthesis of γ , γ -disubstituted unsaturated γ -lactams. **H. Toyama**, a. arit, T. Hashimoto, K. Maruoka
- 2204.** Chiral Brønsted acid catalyzed asymmetric Mannich-type reaction of aldehydes with *N*-carbamate-protected amines. **Y. Aota**, T. Kano, K. Maruoka*
- 2205.** Diaziridination of cyclic secondary amines using haloamide salt. S. Tanaka, S. Minakata*
- 2206.** Iodine-catalyzed diamination of olefins using haloamide salt. S. Minakata*, A. Hirayama, S. Tanaka
- 2207.** Novel NHC-catalyzed synthesis of silyl dienol ethers via 1,4-Brook rearrangement. **H. Amano**, K. Sugimoto, Y. Matsushige*
- 2208.** Chemoselective catalytic oxidation of 1,2-diols to α -hydroxy acids. **M. Shibuya***, K. Furukawa, Y. Yamamoto
- 2209.** Construction of vicinal quaternary chiral centers by asymmetric Mannich type reaction using optically active bis(guanidino)iminophosphorane organosuperbase catalyst. **T. Takeda**, M. Terada*
- 2210.** Development of oxidative kinetic resolution of β -substituted tetralones based on asymmetric α -hydroxylation using guanidine-bisurea bifunctional organocatalyst. **M. Odagi**, M. Sato, M. Yamanaka, K. Nagasawa*
- 2211.** Iodoarene-catalyzed cyclization reactions. **W.J. Moran***
- 2212.** Organocatalysis in confined space for the chemical valorization of carbon dioxide. **V. Dufaud***, B. Chatelet, A. Martinez, J. Dutasta
- 2213.** Novel L-prolinamide based bifunctional chiral organo-catalyst: Synthesis and its application in direct organo-catalytic asymmetric aldol reaction. **P.K. Jaiswal***, D. Dikshit, A. Mishra, S. Chaudhary
- 2214.** Bioinspired organocatalytic enantioselective decarboxylative aldol reaction of malonic acid half thioesters with aldehydes and trifluoromethyl ketones. **J. Sim**, H. Bae, J. Lee, B. List, C. Song*
- 2215.** Thiourea-catalyzed generation of trityl cation species: Application to carbonylene cyclization reaction. N. Nishiyama, R. Horinouchi, H. Kotsuki
- 2216.** Quinonedione-catalyzed oxidative coupling of organomagnesium reagents. **T. Amaya***, R. Suzuki, T. Hirao*
- 2217.** Development of chiral aryl phosphinic acid catalyst and its application to catalytic enantioselective hetero Diels-Alder reaction. N. Momiyama*, T. Narumi, M. Terada*
- 2218.** Asymmetric organocatalytic Michael addition reaction of α -aryl-substituted lactams by phase transfer catalyst: A new short synthesis of (+)-mesembrine. **S. Nunokawa**, M. Minamisawa, H. Kotsuki*
- 2219.** Brønsted acid catalyzed asymmetric silylation of alcohols. **K. Hyodo***, B. List
- 2220.** Efficient enantioselective synthesis of all-carbon-substituted quaternary carbon stereogenic centers through the primary amine-based organocatalytic Michael addition reaction of α -substituted cyclic ketones at high pressure. **R. Horinouchi**, K. Kamei, R. Watanabe, N. Hieda, N. Tatsumi, H. Kotsuki*
- 2221.** Synthesis of architecturally complex block copolymers consisting of oligosaccharide and polyester via organocatalytic ring-opening polymerization. **T. Isono***, T. Satoh*
- 2222.** Asymmetric synthesis of phosphite triesters using chiral Brønsted acid catalysts. **N. Oka***, T. Oshima, K. Ori, T. Sakai, N. Seo, K. Ando
- 2223.** Design and development of C_1 symmetric bis phosphoric acid catalyst. N. Momiyama*, K. Funayama, M. Terada*
- 2224.** Catalytic asymmetric synthesis of anti- α , β -diamino acid derivatives. **S. Izumi**, Y. Kobayashi, Y. Takemoto*
- 2225.** Enantioselective synthesis of [2.2]-paracyclopheanes by chiral phosphoric acid-catalyzed kinetic resolution of PHANOLS. **H. Kishi**, T. Akiyama*, K. Mori
- 2226.** Enantioselective reaction of enamide with azlactone or thiazalone catalyzed by chiral Brønsted acid catalyst. **J. Kikuchi**, N. Momiyama, T. Terada
- 2227.** New and efficient generation of per-fluoroalkyl radicals using highly electrophilic hypervalent iodine(III) reagent under metal-free conditions. **H. Kashiwagi**, K. Maruoka
- 2228.** Migrative cyclization of propargylsulfones using N-heterocyclic carbenes. K. Yamada, Y. Wang*, R. Oriez, Y. Yamaoka, K. Takasu
- 2229.** Organophosphate-catalyzed bulk ring-opening polymerization of cyclic esters. **T. Saito**, T. Isono, K. Tajima, T. Kakuchi, T. Satoh*
- 2230.** Metal-free C–H arylation of arenes with diazonium salts induced by polyaniline. **D. Hata**, T. Amaya, T. Hirao
- 2231.** Efficient photolytic C–H bond functionalization of benzyl compounds with hypervalent iodine(III) reagent. **T. Inada**, K. Maruoka
- 2232.** Flavin-mediated photoinduced thioacetalization of aldehydes. **Y. Arakawa**, T. Miura, K. Minagawa, Y. Imada*
- 2233.** Visible light-induced α -oxyamination of aldehydes with flavin organocatalysts. **T. Tagami**, Y. Arakawa, K. Minagawa, Y. Imada*
- 2234.** Facile preparation of flavinium organocatalysts utilizing cation-exchange resins. **T. Onishi**, Y. Arakawa, K. Minagawa, Y. Imada*
- 2235.** Exploiting intramolecularity: Reaction development using aldehydes as organocatalysts. **A.M. Beauchemin***
- 2236.** Motif for the recognition of phosphonate monoester for the ester hydrolysis catalyst. **A. Shiratori***, N. Kihara
- 2237.** Synthetic study of *trans*-dihydrolycoridine utilizing 1,4-type catalytic asymmetric Friedel-Crafts reaction. **M. Kato**, K. Nagasawa*
- 2238.** Asymmetric Friedel-Crafts alkylation between indoles and α , β -disubstituted acroleins catalyzed by chiral borate salt. **Y. Yagyu**, M. Ueda*, I. Ryu*
- 2239.** A bulky thiyl radical catalyst for [3 + 2] cyclization of vinylaziridine and alkenes. **K. Takino**
- 2240.** Organocatalytic asymmetric Michael reaction of cyclic β -ketoesters and Morita-Baylis-Hillman derivatives bearing a leaving group. **R. Takagi**, E. Fujii, H. Kondo
- 2241.** Highly enantioselective fluorination of α -branched aldehydes with a newly developed chiral primary amine catalyst. **K. Kitahara**, T. Okimi, K. Shibatomi, S. Iwas
- 2242.** Tethered oligopeptides-catalyzed asymmetric conjugate addition reactions. **A. Ueda**, T. Umehiro, R. Eto, M. Tanaka*
- 2243.** N-heteroarenesulfonfonylated cinchona alkaloid amide catalysts: Asymmetric reaction of some nucleophiles with ketimines. **S. Nakamura***
- 2244.** Control of difluorocarbene generation by organocatalyst and its applications. **K. Fuchibe**, Y. Koseki, T. Aono, M. Bando, R. Takayama, J. Ichikawa
- 2245.** Total synthesis of ellagittannins via site-selective sequential functionalization of unprotected glucose. **H. Takeuchi**, K. Mishiro, Y. Ueda, Y. Fujimori, T. Furuta, T. Kawabata*
- 2246.** Enantioselective route to chiral biaryl chloride/lodide by chiral phosphoric acid catalyzed sequential halogenation strategy. **T. Itakura**, K. Mori, T. Akiyama*
- 2247.** First nonenzymatic dynamic kinetic resolution of racemic α -amino acid derivatives by the asymmetric esterification using chiral acyl-transfer catalyst. **E. Tokumaru**, I. Shiomi
- 2248.** Betaine-type electron-transfer catalyst: Design and application. **M. Torii**, D. Uruguchi, T. Ooi
- 2249.** Aerobic alcohol oxidation using AZADOs-NO_x catalysts. **S. Nagasawa**, Y. Osada, Y. Sasano, M. Shibuya, Y. Iwabuchi*
- 2250.** Screening of peptide libraries for discovering efficient amincatalysts. **K. Akagawa**, J. Satou, K. Kudo*
- 2251.** Development of highly active bifunctional organocatalyst having quaternary ammonium as a key functional group. **K. Dan**, A. Kondoh, M. Terada*
- 2252.** Catalytic asymmetric carbon-heteroatom bond-forming reactions at α -position of carbonyl compounds. **Y. Ando**, K. Ohmatsu, T. Ooi*
- 2253.** Water-compatible prolinamide catalysts for stereoselective aldol reaction in aqueous solution. **T. Machinami***, D.M. Miura, T. Fujimoto, M. Tashiro, M. Baba
- 2254.** Chiral binol-based polyethers: Multipurpose chiral organocatalysts. **S. Park**, C. Song*
- 2255.** Asymmetric heterocycle syntheses utilizing multipoint activation by organocatalysts. **K. Asano***, S. Matsubara
- 2256.** Enantioselective desymmetrization of meso-1,2-diols by chiral nucleophilic catalyst containing a 1,1'-binaphthyl unit. **H. Mandai***, H. Yasuhara, K. Fujii, S. Suga*
- 2257.** Planar chiral [2.2]paracyclophane-based phosphine-phenol catalysts bearing exceptionally high reactivity foraza-Morita-Baylis-Hillman reaction. **s. kitagaki***, S. Adachi, A. Furusawa, N. Takenaga, Y. Ohta, C. Mukai
- 2258.** Development of length-selective acylation catalyst using hydrogen bonding between amides. **J. Yabe**, N. Kihara*
- 2259.** Enantioselective Steglich rearrangement of oxindole derivatives and kinetic resolution of secondary alcohols by chiral nucleophilic catalyst containing a 1,1'-binaphthyl unit. **K. Fujii**, H. Mandai, T. Korenaga, S. Suga

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- 2280.** Organocatalytic coupling of carbon dioxide with epoxides: The unexpected boomer effect of fluoroalcohols.
B. Grignard*, S. Gennen, M. Alves, T. Tassaing, C. Jérôme, C. Detrembleur
- 2281.** Organocatalytic asymmetric synthesis of potentially bioactive 3-aminoxindole derivatives.
S.S. Chinni
- 2282.** Diazapane carboxylates in the catalysis of the Cope rearrangement, Diels-Alder cycloaddition and Michael addition.
J. Gleason, D. Kaldre, N. Haggman, F. Larnaud, B. Zank
- 2283.** E/Z-selective asymmetric conjugate addition to electron-deficient internal alkynes.
K. Yamada, D. Uraguchi, T. Ooi*
- 2284.** Guanidinium-hypoiodite catalyzed umpolung type coupling reaction of β -ketooamide with oxindoles.
T. Kato, K. Yasui, K. Nagasawa*
- 2285.** Organocatalysis via halogen–bond interaction.
X. Mi*, S. Guo
- 2286.** Catalytic asymmetric Pictet-Spengler reaction using chiral supramolecular complex.
K. Yamashita, S. Handa, H. Sugimoto*
- 2287.** Stereoselective intramolecular direct cross-aldol and desymmetrization of aliphatic diols enabled by axially chiral aniline.
R. Yella, T. Baba, Y. Tanaka, S. Yamamoto, T. Furuta*, T. Kawabata
- 2288.** DFT study of chiral phosphoric acid catalyzed 1, 4-reduction of α , β -unsaturated ketones.
E. Yamamoto, M. Yamanaka*
- 2289.** Chiral tetraaminophosphonium salts mediated highly regio- and stereoselective 1,6- and 1,8-additions.
K. Yoshioka, D. Uraguchi, T. Ooi*
- 2290.** Theoretical study on chiral bis-phosphoric acid catalyzed asymmetric Diels-Alder reaction.
H. Noda, N. Momiyama, M. Terada, M. Yamanaka*
- 2291.** Synthesis of novel chiral quaternary phosphonium salts with hydrogen-bond donor and their application to asymmetric reactions.
Y. Hidani*, A. Hamasaki, T. ISHIDA, M. Tokunaga

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

New Green Techniques for Medicinal Chemistry (#148)

- Organized by:* W. Zhang, I. Ryu, P. Toy
Presiding: Y. Uozumi, W. Zhang
- 8:00 – 2292.** Access to medically-relevant organoamine scaffolds via palladium-catalyzed decarbonylative allylation.
J.J. Chruman*
- 8:30 – 2293.** Sustainable approaches to palladium-catalyzed cross-coupling reactions.
L. Vaccaro*
- 9:00 – 2294.** Amphiphilic polymeric transition metal catalysts for coupling reactions in water.
Y. Uozumi
- 9:30 – 2295.** Rhodium-catalyzed direct enantioselective alkylation of ketimines: Mechanistic studies and expansion of substrate generality.
T. Ohshima*, K. Morisaki, M. Sawa, R. Yonesaki, H. Morimoto

- 9:50 – 2296.** Green approach to the synthesis of polycyclic compounds through rhodium-catalyzed cyclization of aromatic carboxylic acids.
T. Fukuyama*, S. Maetani, K. Miyagawa, T. Sugimoto, I. Ryu*
- 10:10 – 2297.** Methods for sultam library synthesis.
P.R. Hanson*
- 10:40 – 2298.** Synthesis of highly and diversely substituted heterocycles from alk-3-yn-1-ones (propargyl ketones).
R. Dembinski
- 11:10 – 2299.** Chemical library design based on privileged structure by green chemistry.
H. Liu
- 11:40 – 2300.** Electroactivated heterogeneous catalytic C-H activation at sp³-R₂NC-H and HO-C-H sites: (a) Stereoretentive H/D exchange and (b) Amine alkylation with simple alcohols.
J. Jackson, S. Bhatia, Z. Li

- Hilton Hawaiian Village
Mid-Pacific Center, Coral 2
- Applications of C-H Functionalization (#169)**

- Organized by:* P. Vachal, Z. Shi, C. Li, H. Davies, K. Itami, H. Lebel
- 8:00 – 2301.** C-H functionalization as an enabling methodology for drug discovery.
L. Hamann*
- 8:30 – 2302.** Collaborative approach for C-H functionalization.
H.M. Davies*
- 9:00 – 2303.** C-H functionalization: A transformative technology for drug discovery.
S.W. Krska*
- 9:30 – 2304.** Materials- and biology-oriented C-H activation.
K. Itami
- 10:00 – 2305.** Isoanthine synthesis via Rh(III)-catalyzed intramolecular C-H functionalization.
H. Zhang*
- 10:20 – 2306.** Palladium-catalyzed C-H activation of aliphatic amines.
M. Gaunt*
- 10:50 – 2307.** High-throughput experimentation methods in the development of direct functionalization reactions.
L. Campeau
- 11:10 – 2308.** C-H functionalization symposium.
P.S. Baran
- 11:40 – 2309.** Iridium(III)-catalyzed benzyl amine-directed C-H sulfonamidation of arenes with sulfonyl azides.
M.P. Huestis*, H. Chen

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Strategies and Tactics for Complex Molecule Synthesis (#174)

- Organized by:* C. Forsyth, C. Lee, L. Barriault, J. Cha
Presiding: A.B. Dounay, C. Forsyth
- 8:00** Introduction
- 8:05 – 2310.** Novel tactics for synthesis of functionalized aryl hydroxamic acids.
A.B. Dounay*
- 8:30 – 2311.** Unified synthetic approach toward *ent*-kaurene diterpenoids from *Isodon* species.
L. Zhu, W. Ma, C. Lee*
- 9:00 – 2312.** Synthesis of cephalmyisin A and related bioactive natural products with spiro furanone- γ -lactam core structure.
B. Wang
- 9:25 – 2313.** Total synthesis of aprotinin F.
L. Xiao, M. Jackel, C. Forsyth*
- 9:40 – 2314.** Strategic approaches in the total synthesis of complex natural products.
C. Forsyth*

- 10:10 break**
- 10:20 – 2315.** From alkaloids to terpenoids: Strategies and tactics for the synthesis of polycyclic natural products.
S.E. Reisman

- 10:50 – 2316.** Total syntheses of (-)-supinidine, (-)-isoretronecanol, (+)-elacomine, (-)-kainic acid and efforts toward (D)-dmoic acid using a new annulation strategy.
J.T. Njardarson
- 11:15 – 2317.** Total synthesis of (+)-isoschizogamine.
H. Ueda, A. Takada, H. Fujiwara, K. Sugimoto, H. Tokuyama*
- 11:30 – 2318.** Synthesis of magellaninanetype *Lycopodium* alkaloids using a pyridine functionalization/reduction approach.
V.N. Lindsay*, R.A. Murphy, R. Sarpong
- 11:45 – 2319.** Unified approach toward prenylated indole alkaloid natural products.
E.V. Mercado-Marin, P. Garcia-Reynaga, R. Sarpong

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Cooperative Cocatalysis with Two Different Metals (#270)

- Organized by:* S. Blum, Y. Nakao, S. Chang
- 8:00 – 2320.** Cooperative catalysis with gold and palladium in cross-coupling reactions.
S. Blum*
- 8:40 – 2321.** Pd/Cu complexes: Cooperative and relay catalysis.
m. lesieur, f. lazreg, f. nahra, C. Cazin*

- 9:10 – 2322.** Pd, Cr and Ag in C-H activation: Reactivity and selectivity control in the synthesis of biaryls.
I. Larrosa
- 9:50 Break**
- 10:00 – 2323.** Progress toward dual catalytic, non-directed C-H functionalization.
J.C. Lewis, L. Durak, J. Gair
- 10:40 – 2324.** Cross-coupling reactions by cooperative Pd/Cu catalysis.
K. Semba*, K. Ariyama, R. Kameyama, Y. Nakao*
- 11:10 – 2325.** Dual contemporaneous catalysis for C-C bond formation.
B.M. Trost

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Chemical Glycosylation: Methods and Mechanisms (#306)

- Organized by:* T. Lowary, X. Huang, S. Hung, K. Tanaka
Presiding: X. Huang
- 8:00 – 2326.** Investigations on the chemical and chemoenzymatic synthesis of fragments of O-antigens from a variety of *Shigella* serotypes and species.
L.A. MULARD
- 8:30 – 2327.** Synthesis of immunomodulatory glycoconjugates based on recently developed chemical glycosylation.
Y. Fujimoto*

- 9:00 – 2328.** Simple one-pot regioselective 6-O-phosphorylation of carbohydrates and trehalose desymmetrization.
C. Chang*, C. Wang
- 9:15 – 2329.** Regio- and 1,2-*cis*- α -stereoselective glycosylation utilizing glycosyl acceptor-decorated boronic ester catalyst.
D. Takahashi*, A. Nakagawa, M. Tanaka, K. Toshima*
- 9:30 – 2330.** Development of structurally defined QS saponin-based immune adjuvants.
P. Wang*

- 10:00 Break**
- 10:10 – 2331.** Automated electrochemical assembly for oligosaccharide synthesis.
T. Nakami*, Y. Isoda, K. Takayanagi, N. Sasaki, S. Hayase, T. Itoh*
- 10:40 – 2332.** Control of stereochemistry at anomeric centers via acyclic cation formation: The endocyclic cleavage reaction.
S. Manabe*, Y. Ito
- 10:55 – 2333.** Direct stereoselective glycosidation using unprotected glucose.
Y. Fujimori, H. Takeuchi, T. Furuta, Y. Ueda, T. Kawabata*

- 11:10 – 2334.** Chemoenzymatic synthesis of O-sulfated sialyl Lewis x glycans.
X. Chen*, A. Santra, N. Tasnima, Y. Li, M. Muthana, H. Yu

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4

New Horizon of Process Chemistry by Scalable Reactions and Technologies (#426)

- Organized by:* K. Tomioka, R. Williams, R. Hwu, H. Sajiki, T. Shioiri, N. Yasuda
Presiding: K. Tomioka

- 8:00 – 2335.** Heterogeneous platinum-group metal catalyzed deuterium labeling methods on the basis of C-H activation.
H. Sajiki*, T. Yamada, Y. Sawama, Y. Monguchi

- 8:20 – 2336.** Radical-based C-H functionalization of heteroarenes aimed at late-stage functionalization in drug discovery.
Y. Fujiwara*, P.S. Baran

- 8:40 – 2337.** Practical synthesis of first-in-class MEK inhibitor trametinib (Merkinist®).
H. Abe*, S. Kikuchi, T. Iida, N. Nagashishi, N. Matsumoto, T. Miura, K. Matsumura, N. Seki, T. Ito, H. Kawasaki, T. Inaba

- 8:55 – 2338.** Important catalytic transformations for drug development.
C. Senanayake

- 9:15 – 2339.** Asymmetric synthesis of efavirenz via organocatalyzed enantioselective trifluoromethylation.
N. Shibata*

- 9:35 – 2340.** Application of Shibasaki asymmetric amination to manufacture of ASI-2.
N.N. Bhogle, M. Toshima, S. Watanabe, T. Takasaki*, H. Zhao, M. Filios, J.R. Snoonian, K. Saranteas

- 9:50 Break**
- 10:00 – 2341.** Chemical modification of the 3'-dangling end of dsRNAs for the development of RNA medicines.
Y. Kitade*
- 10:20 – 2342.** Citric acid assisted one-step synthesis for highly dispersed metallic Ru/SiO₂: As-prepared Ru/SiO₂ catalysts for Fischer-Tropsch synthesis.
S. Ishikura, Y. Yoneyama, N. Tsubaki*

- 10:35 – 2343.** Development of analytical standards guaranteed by qNMR.
T. Miura, S. Sugimoto, T. Suematsu, S. Nakao, S. Takaoka, J. Hosoe, H. Nishimura, Y. Kikuchi, T. Katsuhara, T. Yamashita, Y. Yamada, Y. Goda*

- 10:55 – 2344.** Innovative process for carbonates from CO₂.
N. Miyake*, B. NISHIYAMA, M. Shinohata, K. NAKAOKA, Y. KOSUGI

- 11:10 – 2345.** Catalysis in the pharmaceutical industry: Challenges and approaches.
Y. Hsiao*

- 11:30 – 2346.** Magical power of *d*-block transition metals as catalysts for organic synthesis: Principles and examples.
E. Negishi*

Hilton Hawaiian Village
Rainbow Tower, Rainbow 1

Asymmetric Supramolecular Catalysis (#451)

- Organized by:* J. Takacs, S. Moteki, J. Green
Presiding: J. Takacs

8:00 Opening Remarks

- 8:05 – 2347.** Supramolecular concepts in homogeneous catalysis.
B. Breit*

- 8:35 – 2348.** Chirality transfer and amplification phenomena applied to asymmetric catalysis.
M. Raynal*, A. Desmarchelier, X. Caumes, M. Zirmbron, A. Nouar, P. van Leeuwen, C. Thomas, L. Bouteiller

- 9:00 – 2349.** Design and application of chiral supramolecular catalysts based on host-guest interactions.
Q. Fan*

- 9:30 – 2350.** Supramolecularly regulated ligands in asymmetric transformations.
A. Vidal-Ferran*, H. Fernández-Pérez, L. Rovira, M. Vaquero

- 10:00 – 2351.** Rapid identification of optimal ligand for palladium-catalyzed asymmetric allylations.
Y. Hara, K. Ohmatsu, T. Ooi

- 10:20 – 2352.** Switchable rotaxane catalysts.
D. Leigh*

- 10:50 – 2353.** Enantioselective *o*-acylation of meso-1,2-diol with a chiral organocatalyst.
K. XU, T. Iwase, K. Nakazono, T. Takata*

- 11:10 – 2354.** Asymmetric radical processes through supramolecular catalysis.
P. Zhang*

- 11:40 – 2355.** New self-assembly Co(III)-salen catalyst for asymmetric epoxide-opening reactions.
T. Imahori*, Y. Hayashi, M. Doi, M. Watanabe, Y. Kuwahara, S. Kurihara, R. Irie, M. Uchiyama

* Principle Author

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<http://pacificchem.org/onlineprogram>

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Synthetic Modulators of Protein-Protein Interactions (#461)

Organized by: P. Arora, D. Fairlie,
A. Kennan, K. Kumar, S. Sidhu, ,
Presiding: D.P. Fairlie

8:00 Break

8:30 Opening Remarks

8:35 – 2356. Membrane anchored molecules as modulators of protein-protein interactions. **K. Kumar***
9:00 – 2357. Semi-synthetic tRNA complement mediates in vitro protein synthesis. **K.A. Alexandrov**

9:25 – 2358. New encodable chemistry for protein labeling in living cells. **R. Scheck***

9:45 Break

9:55 – 2359. Display platforms for helical ligand discovery. R. Tennyson,
A. Kennan*, B. McNaughton*

10:20 – 2360. Painting proteins blue: β -(1-azulenyl)-L-alanine as a probe of protein-protein interactions. P. Gosavi, Y. Moroz,
G. Caputo, **I. Korendovych**

10:40 – 2361. Design and gram-scale syntheses of small drug-like molecules actings as inhibitors of PP1 helix-mediated protein-protein interactions. **S. Dohmen***,
A. Soeke, R. Opitz, R. Kühne, H. Schmalz

11:00 Break

11:10 – 2362. Small molecule protein–protein interaction surrogates. **A.R. Van Dyke***, J.P. Carolan, A.K. Mapp

11:30 – 2363. Synthetic proteins for modulation of cell signaling. **S.S. Sidhu***

Saturday Afternoon

Hilton Hawaiian Village
Mid-Pacific Center, Coral 5

Designed pi-Electronic Systems: Synthesis, Properties, Theory and Function (#25)

Organized by: T. Kubo, Y. Tobe,
M. Haley, G. Bodwell, K. Wong
Presiding: M.M. Haley

13:00 – 2364. From molecules to materials. **C. Nuckolls***

13:40 – 2365. New aromatic materials for highly efficient small-molecule based organic solar cells. **K. Wong***

14:05 – 2366. Fluorescent and switchable hydrazone-based hydrogel. **I. Abrahamian***, H. Qian

14:30 – 2367. Design and synthesis of novel electron donors and acceptors for high performance organic electronic materials. **Y. Liu***

14:45 – 2368. Brønsted acid promoted polyalkyne benzannulation to synthesize pyrenes, peropyrenes, and graphene nanoribbons. **W.A. Chalifoux**, K.C. Sproul,
C. Sarcinella, W. Yang

15:00 – 2369. Chirality and corannulene. **J. Siegel***

15:25 – 2370. Propellers and scissors – unusual switching motifs in pi-extended isoindolinones. **S. Eisler***, P. Estey,
A. Bubar

15:50 – 2371. Polycyclic aromatic azomethine ylide for the synthesis of planar and bowl-shaped nitrogen-containing PAHs. **S. Ito***, Y. Tokimaru, K. Nozaki*

16:05 – 2372. Synthesis and properties of stable [8]circulene derivatives. **A. Whalley**

16:20 – 2373. Tetracyclopentatetraphenylenes: A non-benzenoid circulene. **Y. Tobe***

16:45 Closing Remarks

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Anion Receptors (#31)

Organized by: B. Hay, F. Pfeffer, B. Wu,
C. Jia, R. Custelcean
Presiding: K. Bowman-James,
F.M. Pfeffer

13:00 – 2374. Anion binding by other anions: Self-assembly in real biological fluids. **F. Hof***, G. Garnett, J. Peña, K. Daze,
M. Ma, L.N. Zakharov

13:30 – 2375. Anion recognition and separation from water by self-assembled guanidinium receptors. **R. Custelcean***

14:00 – 2376. Assembly of anion coordination cages and their inclusion chemistry. **B. Wu***, X. Yang

14:30 Break

14:45 – 2377. System of self-assembled anion-binding $\text{Fe}_4\text{L}_6^{8-}$ cages that adapts to external stimuli. **J.K. Clegg***,
J.R. Nitschke

15:15 – 2378. Computer-aided design of anion receptors. **B. Hay***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 3

Natural Product-based Drug Discovery (#66)

Organized by: B. Baker, R. Kerr, Y. Qin,
D. Uemura, B. Littlefield
Presiding: B.A. Littlefield, D. Uemura

13:00 – 2379. Discovery and development of eribulin (Halaven®), a macrocyclic ketone analog of halichondrin B, for treatment of advanced breast cancer. **B.A. Littlefield***

13:30 – 2380. Industrialization of marine natural product-based drug total synthesis: Crystallization by design in the manufacturing of Halaven. **F. Fang***

14:00 – 2381. Accessing polyketide structures through chemical and biological technologies. **R. Taylor**

14:40 – 2382. Expanding the toolbox: Using the power of synthetic chemistry to devise new cytotoxins configured for use in antibody-drug conjugates. **J. Leighton***

15:10 – 2383. Glimpse into natural product-based drug discovery at Eisai. **M. Postema***

15:30 – 2384. Synthetic studies of manzadins A-C based on diastereoselective hydroxymethylation of chiral nitro compounds. **A. Sakakura***, N. Miyoshi,
T. Kudo

15:50 – 2385. Synthesis of biologically active steroid-derived compounds from an edible mushroom. **T. Nishikawa***, Y. Hirata,
H. Kawagishi

16:10 – 2386. Towards the total synthesis of azaspiracid-3. D. Adu-Ampratwum,
A. Okumu, **N. Kenton**, C. Forsyth

16:20 – 2387. Novel synthetic triterpenoids with powerful anti-inflammatory and cytoprotective activity. **G.W. Grubbe***

16:30 – 2388. Onionin A, a new sulfur-containing compound isolated from onion, impairs tumor development and lung metastasis by regulating macrophage activation. **Y. Fujiwara***, Y. Komohara,
H. Horlad, T. Nohara, M. Takeya

16:40 – 2389. Chemical synthesis of the potent anticancer agent prunostatin A. **M. Chojnacka**, R. Batey*

16:50 Closing Remark

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

New Green Techniques for Medicinal Chemistry (#148)

Organized by: W. Zhang, I. Ryu, P. Toy
Presiding: P.R. Hanson, P.H. Toy

13:00 – 2390. Ionic liquid-mediated improved efficiency of enzymatic kinetic resolution of secondary alcohols. **T. Nishihara**, Y. Matsubara, Y. Fukaya,
T. Nokami, **T. Itoh***

13:30 – 2391. Ionic liquid supported regioselective synthesis of imidazol[5,1-c]quinoxalinines and N-phenylbenzimidazoles via modified Pictet-Spengler reaction. **C. Sun***

14:00 – 2392. Direct construction of C-C and C-S bonds via C-H cleavage. C. Lin,
J. Zhang, B. Wang, M. Yu, **Y. Zhang***

14:30 – 2393. Dealkoxylation cross coupling reactions via the direct functionalization of unactivated $\text{C}_6\text{H}_5\text{O}^-$ bonds. **M. Leidecker**, C. Hsiao, L. Guo,
N. Alandini, M. Rueping*

14:50 – 2394. Study of organic synthesis through aerobic photooxidation. **A. Itoh**

15:20 – 2395. Organic transformations in water via fluorous catalytic systems. **Y. Lam***, W. Ang

15:50 – 2396. Recyclable organocatalysis for organofluorination and other asymmetric synthesis. **W. Zhang***

16:15 – 2397. Reengineering classic organic reactions. **P.H. Toy**

16:40 – 2398. Flash chemistry as a green technique for chemical synthesis. **J. Yoshida**, A. Nagaki

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Applications of C-H Functionalization (#169)

Organized by: P. Vachal, Z. Shi, C. Li,
H. Davies, K. Itami, H. Lebel

13:00 – 2399. Application of C-H functionalization reactions to the synthesis of novel heterocycles. **A.B. Charette**

13:30 – 2400. N-fluorouridomide: Versatile aminating reagents for C–H, C=C and C’C bonds amination. **Q. Zhang**

13:50 – 2401. Iron catalyzed C–H bond amination using high-spin complexes. **T. Bettley***

14:20 – 2402. Iron-catalyzed directed C–H bond activation. **L. Ilies***, E. Nakamura*

14:40 – 2403. PIP bidentate auxiliary in C–H functionalization: Synthetic application and mechanistic studies. **B. Shi***

15:00 – 2404. Rare-earth-catalyzed C–H addition to alkenes and allenes. **Z. Hou***

15:30 – 2405. Catalyst-directed C–H functionalization. **D.A. Nagib**

15:50 – 2406. Pd(II)-catalyzed enantioselective C–H oxidation for the synthesis of arylglycine derivatives. **S. Yang***, X. Wei

16:10 – 2407. Cyclic amines functionalization via sp³C–H bond activation. **C. Bruneau***, M. Achard, B. Sundararaju,
F. Jiang

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Strategies and Tactics for Complex Molecule Synthesis (#174)

Organized by: C. Forsyth, C. Lee,
L. Barriault, J. Cha
Presiding: L. Barriault, J. Gleason

13:00 introduction

13:05 – 2408. Symposium on strategies and tactics in complex molecule synthesis. **P.S. Baran**

13:35 – 2409. Total syntheses of members of the amphiindolin family of marine natural products. **J.S. Clark***, F. Romiti, G. Yang,
A.P. Osnoski, L. Decoutot

14:05 – 2410. Convergent total synthesis of leucosceptrroids and other terpenoids. **D. Ma***, S. Guo

14:35 – 2411. Towards the total synthesis of the tetranortriterpene gedunin. **C.M. Williams***

14:50 – 2412. Concise formal synthesis of haouamine family using palladium-catalyzed alylate cyclization. **H. Tsukamoto***, S. Nakamura, T. Doi*

15:05 break

15:10 – 2413. Progress towards the total synthesis of callosine and related pyrrolidine alkaloids. **M.A. Kerr***, M. Vriesen

15:40 – 2414. Act like molecule transformers: Rapid creation of molecular complexity through strategy/bond disconnections. **G. Liang***

16:10 – 2415. Lewis acid template-catalyzed asymmetric Diels-Alder reaction and its application towards the total synthesis of macrocyclic imine phycotoxins. **J. Ishihara**

16:30 – 2416. Asymmetric total synthesis of (–)-Lingzhiol via a novel type of Rh-catalyzed [3 + 2] cycloaddition. R. Long,
J. Huang, W. Shao, J. Gong, **Z. Yang***

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Cooperative Cocatalysis with Two Different Metals (#270)

Organized by: S. Blum, Y. Nakao,
S. Chang

13:00 – 2417. Synergistic Rh(II)/Pd(0) dual catalysis system for denitrogenative cross-coupling of 1-sulfonyl-1,2,3-triazoles with allyl carboxylates. **z. chen**,
S. Lee

13:30 – 2418. C–C Bond forming reactions by cooperative metal catalysis. **Y. Nakao***

14:10 – 2419. Enhanced additive effects of Zn salts for ruthenium-catalyzed hydrogenation of amides. **T. Higuchi**, Y. Kita,
K. Mashima*

14:40 Break

14:50 – 2420. Cooperative catalysis in deoxygenation processes. **J. Montgomery***

15:30 – 2421. Synthesis of *cis*-1,4-*b-trans*-1,4-polyisoprene using Nd catalyst activated by Mg/Al cocatalysts. **R. Tanaka***

16:00 – 2422. Activation of carbon-cyano bonds using nickel(0) and Lewis acid co-catalysts. **W.D. Jones**, B. Swartz

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Chemical Glycosylation: Methods and Mechanisms (#306)

Organized by: T. Lowary, X. Huang,
S. Hung, K. Tanaka
Presiding: S. Hung

13:00 – 2423. From stereocontrolled glycosylation to expedited oligosaccharide synthesis. **A.V. Demchenko***

13:30 – 2424. In situ glycoconjugation on cell surface: Selective imaging of target using weak glycan/lectin interaction. **K. Tanaka***

14:00 – 2425. Application of h-bond-mediated aglycone delivery (had) in the synthesis of oligosaccharides containing challenging β -manno linkages. **S.G. Pistorio**, A.V. Demchenko

14:15 – 2426. Concise synthesis of the b-ribose-(1–5)-GalNAc moiety in the polysaccharide of *Campylobacter jejuni* NCTC 11168. V.M. Dhurandhare,
G.P. Mishra, **Y. Lam**, C. Wang*

14:30 – 2427. Preactivation-based oligosaccharide synthesis. **X. Ye***

15:00 Break

15:10 – 2428. Iron catalyzed stereoselective glycal aminohydroxylation and diamination reactions: New tools for glycoprotein synthesis. **H. Xu**

15:40 – 2429. Total synthesis of ganglioside PNG-2A found in the starfish *Protoreaster nodosus*. **K. Goto**, T. Suzuki, H. Tamai,
J. Ogawa, H. Ando*, A. Imamura,
H. Ishida, M. Kiso

15:55 – 2430. 2D oligosaccharide syntheses: Recent progress. **X. Liu***

16:10 – 2431. Chemoenzymatic synthesis of heparin and heparan sulfate. **J. Liu***

* Principle Author

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Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 3 & 4
New Horizon of Process Chemistry by Scalable Reactions and Technologies (#426)

Organized by: K. Tomioka, R. Williams, R. Hwu, H. Sajiki, T. Shioiri, N. Yasuda
Presiding: K. Tomioka

13:00 – 2432. New anti-infective agents and a novel delivery strategy. **J. Hwu***, S. Tsay, M. Kapoor, P. Leyssen, J. Neyts
13:20 – 2433. ALIPHASE®: Novel and high efficient liquid-phase peptides and oligonucleotides synthetic method for large scale manufacturing. **D. Takahashi***, T. Inomata, T. Torii
13:40 – 2434. Process chemistry enabling academic basic research: Curved aromatic hydrocarbons. **J. Siegel**
14:00 – 2435. Highly practical new methylation reagent for aldehydes and ketones. **K. Ando***, T. Kobayashi, N. Uchida
14:15 – 2436. Application of engineered biocatalysts in process chemistry. **Y. Hirose***
14:35 – 2437. Parallel and (E)- and (Z)-stereocomplementary synthesis of multisubstituted α,β -unsaturated esters directed for process chemistry: Application to expedited parallel syntheses of all four (E)- and (Z)- Zimeridine and Tamoxifen. **Y. Ashida**, Y. Sato, H. Nakatsuji, Y. Tanabe*

14:50 Break
15:05 – 2438. Cu(II)-catalyzed disymmetrication of dithiomalonates. H. Wauke, K. Matsuo, K. Matsumoto, **M. Shindo***
15:25 – 2439. Practical synthesis of ERK inhibitor GDC-0994 on multikilogram scale. **X. Linghu**
15:40 – 2440. Practical organocatalytic kinetic resolution of a chiral bicyclic ketone for synthesis of a pharmaceutical key intermediate. **Y. Nakamura***, T. Kitawaki, T. Kaneda, K. Nakayama
16:00 – 2441. Development of efficient syntheses of drug candidates and intermediates exploiting novel asymmetric Phase Transfer Catalysed (PTC) reactions. **G.R. Humphrey***
16:20 – 2442. Enantioselective synthesis of chiral amines based on the transfer hydrogenation of ketimines by means of chiral phosphoric acid. **T. Akiyama**
16:40 – 2443. Will new synthetic reagents open the door to the future? **T. Shioiri***

Hilton Hawaiian Village
Rainbow Tower, Rainbow 1
Asymmetric Supramolecular Catalysis (#451)
Organized by: J. Takacs, S. Moteki, J. Green
Presiding: P. Zhang

13:00 – 2444. Supramolecular approaches to control selectivity in transition metal catalysis. **J.N. Reek**
13:30 – 2445. Helical-polymer-based, modular, chirality-switchable chiral catalysts for highly enantioselective asymmetric reactions. **M. Sugimoto***
14:00 – 2446. Discrete metallo-gels based on pincer complexes: A practical platform for molecular visual discrimination and catalysis. **T. Tu***
14:30 – 2447. Bridging the gap between homo and heterogeneous asymmetric catalysis with supramolecular organometallics. **K. Ding**
15:00 – 2448. Asymmetric catalysis in nanopores: Bridging homogeneous and heterogeneous catalysis. **Q. Yang***
15:30 – 2449. Enantioselective hydroformylation by a Rh-catalyst entrapped in a supramolecular metallocage. C. García-Simón, R. Gramage-Doria, S. Raouf moghaddam, T. Parella, D. Costas, X. Ribas, J.N. Reek

15:50 – 2450. Design principles of chirally modified metal catalysts for heterogeneous asymmetric hydrogenations derived from *operando* spectroscopic studies. **F. Meemken***, K. Hungerbühler, A. Baiker

16:10 – 2451. Metallacrown ether catalysts for supramolecular asymmetric hydrogenation. **Y. He***, F. Song, Q. Fan*
16:30 – 2452. Site-selective supramolecular catalysts for catalytic asymmetric hydroboration. K. Toyama, K. Marichev, **J. Takacs***

16:50 Closing Remarks

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Synthetic Modulators of Protein-Protein Interactions (#461)

Organized by: P. Arora, D. Fairlie, A. Kennan, K. Kumar, S. Sidhu, , *Presiding:* S.S. Sidhu

13:00 Opening Remarks
13:05 – 2453. Drugging the undruggable: The inhibition of MYC. **K.D. Janda***
13:30 – 2454. Fragment screening and drugability assessment for the CBP/p300 KIX domain via protein observed ^{19}F NMR. **W.C. Pomerantz***, C.T. Gee, E.J. Koleski

13:50 – 2455. Macro cyclic inhibitors of human histone deacetylase enzymes. **C.A. Olsen***

14:10 Break

14:20 – 2456. Applying structural diverse small protein libraries to the investigating of protein-protein interactions. **K. Deshayes***

14:45 – 2457. On-bead screening of proteo-mimetics libraries for discovery of protein-protein interaction modulators. **H. Lim***

15:05 – 2458. Small molecules that modulate protein assemblies. **M. Uesugi**

15:30 Break

15:40 – 2459. Controlling protein interaction networks with synthetic binding protein. **S. Koide**

16:05 – 2460. Synthetic proteins inhibit protein-protein interactions involving the oncoprotein gankyrin and modulate disease-relevant biochemical processes. **B. McNaughton***, A.M. Chapman

16:25 – 2461. RaPID way to discover PPI agonists and antagonists. **H. Suga***

Saturday Evening

Hawaii Convention Center
Halls I, II, III

New Green Techniques for Medicinal Chemistry (#148)

Organized by: W. Zhang, I. Ryu, P. Toy

Poster Session

19:00 – 21:00

2462. Iodide as an activating agent in acylation reactions. **C.S. Jones***, R.J. Wakeham, S.D. Bull, J.M. Williams

2463. Catalytic chemoselective conjugate addition of alcohols over amines. **R. Yazaki***, S. Uesugi, Z. Li, T. Ohshima*

2464. Quantitative determination of acetaminophen, acetilsalicylic acid, cetrizine dihydrochloride, and fenofenadine hydrochloride by quantitative NMR technique. **S. Kumar***, M. Villanueva, J.F. Zukic, C. Flemming, S. Kumar, G.K. Webster

2465. Microwave-assist synthesis of hydroxamic acid derivatives as histone deacetylase inhibitors. **H. Shin***

2466. Catalytic asymmetric cyclization of ω -carboxy-substituted allylic alcohols to the lactone. **Y. Suzuki**, S. Tanaka, M. Kitamura*

2467. Design and synthesis of quinolone-based radioprotecting agents. **S. Aoki**, Y. Nishi, S. Ariyasu, A. Morita, W. Bing

2468. Synthesis and structure of hypervalent iodine(III) reagent containing phthalimidate and its application to oxidative amination reaction. **K. Kiyokawa**, T. Kosaka, S. Minakata*

2469. Hypervalent iodine(III)-mediated de-carboxylative functionalization of β,γ -unsaturated carboxylic acids. **T. Kojima**, K. Kiyokawa, S. Minakata*

2470. Ritter-type C–H amination using *N*-hydroxyphthalimidate and iodic acid. **K. Takemoto**, K. Kiyokawa, S. Minakata*

2471. Sustainable synthesis of 2-pyrrolidon-2-one catalyzed by a polymer supported acid in solvent-free conditions. **D. Lanari**, M. Curini, L. Vaccaro

2472. Four-component radical coupling reaction using CO and sulfonyl oxime ethers. **M. Sasano**, S. Sumino, T. Fukuyama, I. Ryu*, A. Jacquet, F. Robert, **L. Landais***

2473. Photocatalytic N-methylation of amines with methanol for medicinal chemistry. **Y. Morioka**, L. Wang, V.N. Tsarev, J. Caner, Q. Wang, R. Ushimaru, A. Kudo, H. Nakao, S. Saito

2474. Synthesis of chiral 1,2,3-triazolium ionic liquid. **J. Ryu***

2475. Photoinduced metal-free aminocarbonylation of aryl iodides. **A. Sato**, T. Kawamoto, I. Ryu*

2476. Tetraethylorthosilicate as a mild dehydrating reagent for the synthesis of *N*-formamides with formic acid. **K. Matsuda**, Y. Nishikawa, N. Ukai, E. Nakamura, W. Adachi, R. Satoh, S. Moriguchi, O. Hara

Hawaii Convention Center
Halls I, II, III

Applications of C–H Functionalization (#169)

Organized by: P. Vachal, Z. Shi, C. Li, H. Davies, K. Itami, H. Lebel

Poster Session

19:00 – 21:00

2477. Rhodium(III)-catalyzed direct alkenylation of 1,3-dithiane-protected arenecarb-aldehydes. **Y. Unoh**, K. Hirano, T. Satoh, M. Miura

2478. Regioselective C–H dual functionalization of indoles using hypervalent iodine(III). **K. Moriyama**, H. Togo

2479. Cu(II)-catalyzed oxidative esterification of 2-carbonyl substituted phenols with ethers acyl equivalents. **S. Han***

2480. Chemo- and site-selective aerobic oxygenation of sp^3 C–H bonds of alcohols using *N*-oxyl radical directing activator. **K. Osaki***, J. Ozawa, J. Ni, M. Tashiro, M. Kanai

2481. Direct arylation polymerization toward sustainable high performance polymer solar cells. **A. Dudnik**, T.J. Aldrich, N.D. Eastham, R.P. Chang*, A. Faccetto*, T.J. Marks*

2482. C–H activation with copper containing silica-based metal complexes . **A. Karkamkar***

2483. Synthesis of benzofuro[3,2-b]pyridines via Pd-catalyzed dual C–H activation of 3-phenoxy pyridine 1-oxides. **P. Li***

2484. Catalytic enantioselective oxidative C–H functionalization of structurally diverse heterocycles. **Z. Meng**, X. Liu, S. Sun, L. Liu*

2485. Rhodium-catalyzed silylation of C–H bonds in aromatic amides with α,β -unsaturated lactones. **K. Shibata**, N. Chatani*

2486. Electron-deficient (n^5 -cyclopentadienyl)rhodium(III) complex-catalyzed C–H Bond functionalization reactions under ambient conditions. **Y. Shibata**, Y. Hoshino, Y. Takahama, M. Fukui, M. Yamazaki, E. Kudo, K. Tanaka*

2487. One-pot oxidation and direct C–H silylation of arylmethanols catalyzed by iridium complexes with *N*-xylyl-*N'*-methylperimidine carbene. **H. Tsurugi**, G. Choi, R. Rochat, K. Mashima*

2488. Powerful Mo^{IV} reagent for the selective oxidative coupling reaction. **S.R. Waldvogel***

2489. Oxidative cross-coupling of pyridine N-oxides and ethers between C(sp²)-H/C(sp³)-H bond under transition-metal-free conditions. **L. Wang***

2490. Development of catalytic asymmetric direct-type 1,4-addition reactions of simple amides and esters. **Y. Yamashita**, H. Suzuki, I. Sato, S. Kobayashi*

2491. Copper-catalyzed direct α -ketoesterification of propiophenes with acetophenones via C(sp³)-H oxidative cross-coupling. **X. Zhang***

2492. Hydroamination of olefin catalyzed by silica supported metalaziridine: Evidences for the mechanism. **J. Bassett**, B. Hamzaoui, j. pelletier, M. El Eter, S. ouldchikh

2493. Palladium-catalyzed β -arylation of oximes with diaryliodonium salts through activation of inert C(sp³)-H bond. **C. Chen**

2494. Enantioselective C–H arylation for chiral phosphine synthesis. **Z. Lin**, W. Wang, S. Yan, **W. Duan***

2495. Nickel-catalyzed direct borylation of C–H bonds in arenes and indoles. **T. Furukawa**, M. Tobisu*, N. Chatani*

2496. Iron-catalyzed C–H amination of aniline derivatives. **Y. Aoki***, R. Imayoshi, T. Hatakeyama, H.R. Takaya, M. Nakamura

2497. Direct arylation of thiocarbonylated compound catalyzed by Pd-phenanthroline complexes. **T. Yamauchi***, T. Murai, F. Shibahara

2498. Cobalt-catalyzed sp³ C–H amination utilizing aryl azides. **C.E. MacBeth***, S.B. Blahey, N.M. Welyd, O. Villanueva

2499. Unprecedented alkali metal amide-catalyzed formal C(sp³)-H bond activation. **W. Bao**, H. Kossen, U. Schneider

2500. Total synthesis of myricin and its analog using Rh(II)-catalyzed C–H amination and the following alkylation. **N. Noda**, K. Ubukata, W. Niu, T. Fujiwara, H. Nambu, T. Yakura

2501. Silver-catalyzed C–H trifluoromethylation of arenes using trifluoroacetic acid as the trifluoromethylating reagent. **G. Shi**

2502. Ruthenium-catalyzed ortho-selective arylation of sterically-congested C–H bonds of aromatic ketones. **M. Miyake**, Y. Ogihara, T. Kochi, F. Kakuichi*

2503. *para*-Selective C–H borylation of benzene derivatives. **Y. Saito**, Y. Segawa*, K. Itami*

2504. Palladium-catalyzed cross dehydrogenative coupling between unactivated C(sp³)-H bonds in aliphatic amides and benzylic C–H bonds in toluene derivatives. **T. Kubo***, Y. Aihara, N. Chatani

2505. Palladium-catalyzed C–H ethoxycarbonyl/difluoromethylation of electron-rich heteroarenes promoted by ligand. **C. Shao**

2506. Inverse micelle templated mesoporous manganese oxide as an efficient heterogeneous catalyst for solvent free oxidation of C–H bond. **S. Biswas***, K. Mullick, S. Chen, S. Suib

2507. Oxidative alkenylation and cyclization of *N*-benzyltriflamides with olefins via C–H bond activation under rhodium catalysis. **S. Han***

2508. Oxidative olefination of 1,2-disubstituted arylhydrazines with alkene under rhodium catalysis. **M. Choi***

2509. Pd(II)-catalyzed decarboxylative acylation of highly substituted indolines with α -keto acids via C–H bond activation. **M. Choi***

2510. Pd(OAc)₂-catalyzed lactonization of aromatic acetamides involving oxidation of C–H bonds. **T. Igarashi**, M. Moguchi, T. Uemura, N. Chatani

* Principle Author

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<http://pacificchem.org/>

onlineprogram

- 2511.** Pd(II)-catalyzed oxidative C7-acylation of indolines at the C7-position with aldehydes or alcohols. **A. Kyung***
- 2512.** Pd-catalyzed dual C–H activation of bis-alkynes and biaryl alkynes. **T. Jin***, J. Zhao, N. Asao, Y. Yamamoto
- 2513.** Regioselective chlorination of benzamide derivatives using a combination of anodic oxidation and palladium-catalyzed cleavage of aromatic carbon–hydrogen bonds. **M. Konishi**, K. Tsuchida, T. Kochi, F. Kakuchi*
- 2514.** Rh(III)-catalyzed selective C7-allylation of indolines with allylic carbonates at room temperature. **T. Jeong***
- 2515.** Rh(III)-catalyzed selective C-H allylations of indolines and indoles with 4-vinyl-1,3-dioxolan-2-one at room temperature. **M. Choi***
- 2516.** Rh(III)-catalyzed selective cyanation of C–H bonds of indolines and indoles with an easily accessible cyano source. **T. Jeong***
- 2517.** Rhodium-catalyzed *ortho*-selective C–H α -acylalkylation of arenes using cyclic alkanyl carbonates. **S. Onodera**, Y. Hara, T. Kochi, F. Kakuchi*
- 2518.** Rhodium-catalyzed direct silylation of C–H bonds in pyridine derivatives at the 3-position. **Y. Fukumoto***, **M. Hirano**, N. Chatani
- 2519.** Rhodium-catalyzed oxidative C2-alkylation of indoles with alkynes via C–H bond activation. **A. Kyung***
- 2520.** Rhodium-catalyzed oxidative C2-olefination of N-substituted indole and pyrroles with a range of alkenes via C–H bond activation. **T. Jeong***
- 2521.** Ru(II)-catalyzed oxidative allylation, croylation, and prenylation of aromatic and α , β -unsaturated carboxamides with allylic carbonates. **S. Han***
- 2522.** Ruthenium(II)-catalyzed selective C–H amination of xanthones and chromones C–H bonds with sulfonyl azides. **A. Kyung***
- 2523.** Efficient synthesis of 4-substituted tryptophan derivatives via Ir-catalyzed C–H bond activation: Total synthesis of *cis*-clavicipit acid. **M. Ito**, Y. Tahara, T. Shibata*
- 2524.** Direct hydroxylation and amination of arene via deprotonative cupration. **K. Shimjo**, N. Tezuka*, S. Komagawa, K. Hirano, R. Takita, M. Uchiyama
- 2525.** Asymmetric synthesis of fused piperidine derivatives by the domino internal redox process. **R. Isogai**, K. Mori, T. Akiyama*
- 2526.** Cu-catalyzed oxidative C–H/C–O cyclization of binaphthols using air as the sole oxidant: Efficient synthesis of PXX derivatives. **T. Kamei***, **M. Uryu**, T. Shimada*
- 2527.** Construction of spirocyclic skeleton by intramolecular redox cyclization/Friedel-Crafts reaction sequence. **E. Kitamura**, K. Mori, T. Akiyama
- 2528.** Direct coupling of oxazoline ring with aryl halides for the preparation of chiral oxazoline-containing ligands. **Y. Nishikawa**, **S. Kawaguchi**, K. Takemoto, T. Ishiguro, K. Miwa, O. Hara
- 2529.** Palladium-catalyzed synthesis of dibenzothiophenes via the cleavage of carbon–hydrogen and carbon–sulfur bonds. **M. Tobisu***, **Y. Masuya**, K. Baba, N. Chatani
- 2530.** Stereoselective construction of tetrahydropyrimidinone derivatives with intramolecular allylic C–H amination. **Y. Nishikawa**, **A. Ito**, Y. Kato, S. Maegawa, Y. Yatsuhashi, E. Niwa, E. Kuze, O. Hara
- 2531.** Cross-coupling hydrogen evolution reaction by visible light catalysis. **Q. Meng***, X. Gao*, J. Zhong, **C. Tung**, L. Wu*
- 2532.** Enantioselective synthesis of planar chiral benzosiloferrocenes via Rh(I)-catalyzed intramolecular direct C–H silylation. **T. Sasaki**, T. Shizuno, T. Shibata*
- 2533.** Rhodium-catalyzed reaction of C–H bonds in aromatic amides with styrenes. **T. Yamaguchi**, K. Shibata, N. Chatani*

- 2534.** Pd(II)-catalyzed alkoxylation of unactivated C(sp³)–H and C(sp²)–H bonds using a removable directing group: Efficient synthesis of alkyl ethers. **F. Hu**
- 2535.** DCCR. **W. Su**
- 2536.** Photocatalyzed site-selective C–H/C–C conversion of functionalized alkanes. **K. Yamada**, M. Okada, T. Fukuyama, D. Ravelli, M. Fagnoni*, I. Ryu*
- 2537.** Synthesis of chromane derivatives: Palladium-catalyzed cyclization of alkynyl aryl ethers with strained alkenes via C–H activation. **T. Kodama**, Y. Minami*, T. Hiyama*
- 2538.** Nickel catalyzed cross-coupling reactions of o-carboranyl with aryl iodides: Facile synthesis of 1-aryl-o-carboranes and 1,2-diaryl-o-carboranes. **C. Tang**, Z. Xie*
- 2539.** C–H alkylation for 2-substituted pyridine N-oxides by a cationic iridium(I) catalyst. **H. Takano**, T. Shibata*
- 2540.** Heterogeneously catalyzed aerobic oxidative coupling of aryl amines. **K. Matsumoto**, K. Dougomori, S. Tachikawa, M. Shindo
- 2541.** Selenium dioxide-mediated twofold C–H activation of phenols. **T.J. Quell***, S.R. Waldvogel, K.M. Dyballa, R. Franke
- 2542.** Palladium-catalyzed C–H arylation with aryl sulfides. **S. Otsuka**, H. Yorimitsu*, A. Osuka
- 2543.** Aromatic metamorphosis of dibenzofurans to triphenylenes. **Y. Kurata**, S. Otsuka, N. Fukui, **H. Yorimitsu***, A. Osuka
- 2544.** Stereoselective construction of imidazolidinone derivatives with intramolecular allylic C–H amination. **Y. Nishikawa**, **H. Tsurumi**, S. Kimura, N. Yamazaki, N. Akada, O. Hara
- Hawaii Convention Center
Halls I, II, III
- Strategies and Tactics for Complex Molecule Synthesis (#174)**
- Organized by: C. Forsyth, C. Lee, L. Barria, J. Cha
Presiding: A.M. Hardman-Baldwin, J.M. Wieting
- Poster Session**
19:00 – 21:00
- 2545.** Synthetic study on isoflavanoids based on 1,2-rearrangement strategy. **K. Nakamura**, K. Ohmori, K. Suzuki*
- 2546.** Total synthesis of cardiotropetanine. **Y. Nishiyama**, S. Yokoshima, T. Fukuyama
- 2547.** Synthesis and biological evaluation of fully synthetic C5-oxatetracyclines. **F. Liu**, P. Wright, A.G. Myers*
- 2548.** Nanomole-scale high-throughput chemistry for the synthesis of complex molecules. **A. Buitrago Santanilla***, E.L. Regalado, T. Pereira, M. Shevlin, K. Bateman, L. Campeau, J. Scheneewels, S. Berrett, Z. Shi, P. Nantermet, Y. Liu, R. Helmy, C. Welch, P. Vachal, I. Davies, T. Cernak, S. Dreher
- 2549.** Functionalized pyrans by stereospecific and regiodivergent Suzuki–Miyaura cross-coupling of dihydropyranyl boronates. **T.I. Rybak**, D. Hall*
- 2550.** Development of asymmetric dearomatic cyclization for synthesis of hinckdenine. **A. K. Douki**, H. Ono, J. Shimokawa, T. Fukuyama*, M. Kitamura*
- 2551.** TiO₂-directed (3+2) cycloadditions of benzynes for the regioselective synthesis of functionalized benzo-fused heterocycles. **T. Ikawa**, **h. kaneko**, S. Masuda, S. Arai*
- 2552.** Regio- and stereoselective halothiolation of alkynes catalyzed by palladium and iron. **M. Iwasaki**, T. Fujii, A. Yamamoto, N. Michihiro, K. Nakajima, Y. Nishihara*
- 2553.** Total synthesis of tetracenomycin C. **S. Sato**, Y. Hashimoto, H. Takikawa, K. Suzuki*
- 2554.** Functional porphyrinoid conjugates – complex organic systems toward functional materials. **H. Ngo***
- 2555.** Asymmetric total synthesis of (+)-en-gelhaarquinone via Rh-catalyzed asymmetric Michael addition and thiol-mediated reductive cyclization. **T. Fukazawa**, S. Hori, Y. Ando, K. Ohmori, T. Hayashi, K. Suzuki
- 2556.** Advances in thermal and photochemical Cu(I)-catalyzed macrocyclic Sonogashira-type cross-couplings. **J. Santandrea**, A. Bédard, C. Minozzi, S. Collins*
- 2557.** Synthetic strategy of highly oxygenated diaryl ethers resulting in ellagitanins. **H. Yamada***, T. Hirokane, Y. Hirata, T. Ishimoto, K. Nishii
- 2558.** Total synthesis of (-)-sphingofungin E using asymmetric bromolactonization. **K. Ikeuchi**, M. Hayashi, T. Yamamoto, M. Inai, T. Asakawa, Y. Hamashima, T. Kan*
- 2559.** Synthesis and stereochemical study of decarestrictines G, H, and J. **R. Katsuta**, S. Fujikawa, N. Masada, S. Ueda, Y. Shimodaira, A. Yajima, T. Nukada
- 2560.** Synthetic studies on tetrodotoxin model compound using mercury(II) triflate-catalyzed novel cycloisomerization. **T. Maruyama**, S. Kikuchi, T. Koyama, K. Nishikawa, Y. Tachi, Y. Morimoto*
- 2561.** Highly chemoselective aerobic oxidation of amino alcohols into amino carbonyl compounds using AZADO/copper catalysis. **Y. Sasano**, S. Nagasawa, N. Kogure, M. Shibuya, J. Park, Y. Iwabuchi*
- 2562.** 2-Naphthylmethoxymethyl (NAPOM) group - a new member of the BOM protective group family. T. Sato, T. Oishi, K. Torikai*
- 2563.** Enantioselective syntheses Sch642305 and Glabramycin B, antibacterial 10-membered lactones fused with 4-oxogenated cyclohexanone. **K. Ishigami***, M. Yamamoto, R. Katsuta, H. Watanabe
- 2564.** Synthetic study of gymnocin-A using an oxiranyl anion strategy. **T. Sakai**, S. Matsushita, S. Arakawa, K. Mori, M. Tanimoto, A. Tokumasu, T. Yoshida, Y. Mori*
- 2565.** Biomimetic total synthesis of (+)-cytoprolide A via a hetero-Diels–Alder reaction. **K. Takao***, S. Noguchi, S. Sakamoto, K. Yoshida
- 2566.** Metal-free carbon dioxide fixation. **A.M. Hardman-Baldwin**, A.E. Mattson
- 2567.** One-pot preparation of tetralin derivatives by indium(III)-catalyzed reductive iodination and intramolecular cyclization of 3-benzoylpropionic acids. **T. Kobayashi***
- 2568.** Asymmetric total syntheses of tirandamycins by utilizing cinchona alkaloid catalyzed Morita–Bailly–Hillman reactions. **H. Yoshimura**, K. Takahashi, J. Ishihara, S. Hatakeyama*
- 2569.** Synthesis of the 5,6-epoxyisoprostane E2 part of PEIPI through aldol reaction of the α -bromocyclopentanone. **Y. Kobayashi**, H. Kawashima
- 2570.** Synthesis of welwitindolinone alkaloids by Pd(0)-catalyzed tandem intramolecular enolate coupling. **K. Komine**, Y. Nomura, C. Pieri, K. Takahashi, J. Ishihara, S. Hatakeyama*
- 2571.** Unified total synthesis of rianoids. **M. Kohshima***, M. Nagatomo, M. Inoue
- 2572.** Strategic coupling of chiral fragments via kinetic resolution: Total synthesis and structure revision of vallartanone A. **D. Kundu**, D. Ward*
- 2573.** Tetracyclic compounds through single operation using TMM diyl intermediates: Application to the total synthesis of Waiohensene. **H. Lee**, H. Lee
- 2574.** Substrate-controlled total synthesis of (+)-chamavarin via triple intramolecular Si₂ alkylations. **J. Lee***
- 2575.** Stereoselective total synthesis of (-)-protoemetinol. **C. Lim**, H. Moon, J. Sim, Y. Suh, K. Kim
- 2576.** Novel synthesis of zanamivir. **L. Lin***, J. Fang
- 2577.** Synthetic study on (-)-Kainic acid using SmI₂. **N. Miyano**, T. Umezawa, F. Matsuda
- 2578.** Synthetic studies of perforatumone: Construction of a unique bridged bicyclic skeleton. **T. Nakajima**, K. Yoshida, K. Takao*
- 2579.** Synthetic studies of JK-ring system of yesotoxin. **K. Nishida**, M. Miyazawa, H. Yokoyama*
- 2580.** Total syntheses of lepadiformines using Hg(OTf)₂-catalyzed novel cyclomeration. **K. Nishikawa**, K. Yamauchi, S. Kikuchi, S. Ezaki, T. Koyama, T. Kodama, Y. Tachi, Y. Morimoto*
- 2581.** Development of highly Z-selective reagents for olefinations using pentacoordinated phosphoranes. **W. Ohata**, S. Kojima, Y. Yamamoto
- 2582.** Synthesis of jiadifenin using Mizoroki–Heck and Tsuji–Trost reactions. **K. Harada**, A. Imai, M. Kubo, H. Hioki, Y. Fukuyama*
- 2583.** Total synthesis of Laurallene. **T. Okada**, F. YOSHIMURA, K. Tanino
- 2584.** Preparation of 1,4-benzooxanes by iron(III)-catalyzed cycloaddition of o-quinone. A. Kuboki*, **Y. Okazaki**, K. Morita, M. Okano, Y. Suezaki, S. Ohira*
- 2585.** Iodonium-mediated dearomatic cyclization/Diels–Alder tandem of a chiral ynamide toward diastereoselective construction of bridgehead-spiro system. **T. Okitsu***, C. Murai, A. Wada
- 2586.** Preparation of highly functionalized and stable o-quinones. A. Kuboki*, **R. Ookuma**, K. Suzuki, C. Honda, K. Morita, S. Ohira*
- 2587.** Nitrimines as reagents in metal-free cross coupling reactions. V.W. Angeles-Dunham*, **A. Curtze**, A.E. Mattson
- 2588.** Asymmetric synthesis of (-)-horsfiline, (+)-coerulescine, and (3S,4R)-(-)-Elacomine through chiral auxiliary induction. **O. Forero Doria***, L. S. Santos
- 2589.** Total synthesis of cavicularin using Pd-catalyzed Ar–Ar coupling and Suzuki–Miyaura reaction. **Y. Fukuyama***, K. Makino, K. Harada, M. Kubo, H. Hikio
- 2590.** Total synthesis of jujuylene: Cycloclooctanoid synthesis from oxipolyrrylum ion dimerization reaction. **S. Geum**, H. Lee*
- 2591.** Eight-step synthesis of chaixine B based on a proposed biosynthetic pathway. **Y. Hirata**, T. Nishikawa
- 2592.** Total synthesis of madeirolide A. **S. Hwang**, I. Baek, C. Lee*
- 2593.** Studies directed toward the total synthesis of brasiliardin A. **R. Itoh**, M. TORIZUKA, G. MORI, F. YOSHIMURA, K. Tanino
- 2594.** Synthetic studies on cylindradine B. **Y. Kamijoh**, M. Iwata, K. Nagasawa*
- 2595.** Total synthesis of (+)-ceratopicanol synthesis: Comparison between consecutive Pd mediated cyclization and ruthenium catalyzed enyme radical cyclization. **R. Kim**, H. Lee*
- 2596.** Asymmetric sequential reaction for the synthesis of α -aryl- β -hydroxy amides. **S. Shin**, E. Baek, D. Ryu*
- 2597.** Traceless C–C bond formation via tandem alkylation and retro-ene reactions using heterocyclic sulfones. **Y. Chae**, H. Park, C. Lee*
- 2598.** Synthetic studies of palau'samine. **M. Iwata**, T. Imaoka, H. Matsuo, K. Nagasawa*

* Principle Author

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2599. Synthetic study of FD-891 and FD-892. **A. Kawamura***, T. Itagaki, Y. Miyazaki, K. Yahata, E. Kwon, Y. Iwabuchi, N. Kanoh

2600. Studies toward the total synthesis of polediene. **S. Kim**, S. Kim, R. Matunas, C. Lee*

2601. Catalytic asymmetric insertion of aryl-diazoalkane and diazoesters into C–H bond of aldehydes. **B. Kang**, D. Nam, G. Hwang, D. Ryu*

2602. Synthetic study of chloropupukeanin by a biomimetic Diels–Alder/carbonylne cascade. **T. Suzuki***, Y. Miyajima, K. Suzuki, S. Kobayashi, K. Tanino

2603. Catalytic asymmetric cyclopropanation with α -alkyl diazo compounds and substituted acroleins: Its application to total synthesis of Hamavellone A and B. **S. Shim**, J. Kim, D. Ryu*

2604. Efficient synthesis of polycyclic aromatic hydrocarbons using ruthenium-catalyzed C–O arylation. **Y. Suzuki**, T. Kochi, F. Kakuchi*

2605. Total synthesis of marinomycin A based on a direct dimerization strategy. **N. Tatsuya***, M. Kondo, K. Takeshita, K. Takahashi, J. Ishihara, S. Hatakeyama

2606. Studies toward total synthesis of nigricanose-A and determination of its absolute stereochemistry. **T. Tsunoda**, K. Fujiwara*, S. Okamoto, Y. Kuriyama, W. Nojo, N. Kinashi, R. Katono, T. Suzuki

2607. Synthesis of 1-amino-25-hydroxy vitamin D₃. **K. Usuda**, R. Asano, M. Watanabe, M. Uesugi*, K. Nagasawa*

2608. Knoevenagel condensation of aldehydes and activated methylenes using indium chloride with acetic anhydride as a promoter. **K. Takahashi**, T. Kitazawa, Y. Ogiwara, N. Sakai

2609. Synthesis of a [2]rotaxane from a less sterically hindered phenanthroline-copper complex. **Y. Yamazaki***, T. Ohkubo, T. Yokoyama, Y. Mutoh, R. YAMASAKI, T. Kasama, S. Saito

2610. Asymmetric anion binding catalysis with chiral silanediols. J.M. Wieting, T.J. Fisher, A.G. Schafer, **M.D. Visco**, J. Gallucci, A.E. Mattson*

2611. Synthetic studies of 11-saxitoxinethanoic acid. **C. Wang**, M. Oki, T. Nishikawa, K. Nagasawa*

2612. Synthetic studies on muironolide A. **K.E. Rosa Pagan**, C.M. Clay, K. Cunningham, I. Modolo, C. Forsyth*

2613. Synthetic studies on the JKRL-ring of ciguatoxin-3C. **K. Fujiwara**, **T. Saito**, Y. Sano, R. Katono, T. Suzuki

2614. Synthetic studies toward (–)-calophycoic acid A: Construction of all-carbon quaternary stereocenters by allylboration of chiral aldehydes. **A. Sakama**, K. Yoshida, K. Takao*

2615. Synthetic studies on the ABCDEF-ring of ciguatoxin-3C. **T. Sato**, K. Fujiwara, Y. Nomura, R. Katono, T. Suzuki

Hawaii Convention Center
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Cooperative Cocatalysis with Two Different Metals (#270)

Organized by: S. Blum, Y. Nakao, S. Chang

Poster Session
19:00 – 21:00

2616. Development of hydroxyapatite-supported ruthenium–vanadium bimetallic catalyst for highly selective reduction of amides to amines. **K. Miyagawa**, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa, K. Kaneda*

2617. Ir catalyzed asymmetric tandem reaction of meso-diols. **T. SUZUKI***, I. Ismiyarto, D. Zhou, K. Asano, H. Sasai

2618. Cooperative catalysis of Cu and Mn in aerobic oxidative coupling of terminal alkynes. **S. Biswas***, A.R. Rossi, S. Suib

Hawaii Convention Center
Halls I, II, III

Chemical Glycosylation: Methods and Mechanisms (#306)

Organized by: T. Lowary, X. Huang, S. Hung, K. Tanaka
Presiding: X. Huang, S. Hung, T. Lowary, K. Tanaka

Poster Session
19:00 – 21:00

2619. Oligosaccharides synthesis using silicon bulky protecting group.

T. Matsumoto, R. Ito, R. Konose, T. KOYAMA, K. MATSUOKA, K. Hatano

2620. α -Selective ribofuranosylation using ribofuranosyl iodides as glycosyl donors. **N. Oka***, R. Kajino, K. Ando

2621. Reactivity and stereoselectivity of glycosylation using glycosyl acceptor having thioether groups near to alcohol.

M. Kobayashi, M. Tamura, A. Ezawa, Y. Nishida, H. Dohi*

2622. Synthesis of selenum-containing fucose derivatives and their application for the X-ray structural analysis of fucose-binding lectin from *Aspergillus oryzae*.

J. Shimabukuro, H. Makyo, T. Suzuki, H. Ando*, Y. Yamada, H. Ishida, S. Wakatsuki, R. Kato, M. Kiso

2623. Efficient synthesis of Rhamnan sulfates with repeating 1,2- α -linkages unit and alternating 1,2- and 1,3- α -linkages by using disaccharide building blocks. **H. Tanaka***

2624. Stereoselective synthesis of antiherpesvirus sialyl T_N-glycopeptides.

K. Kakita*, N. Hatori, A. Furukawa, M. Anada, H. Nambu, K. Maenaka, S. Hashimoto

2625. Design and synthesis of thioglycoside donors having electron-donating groups for the efficient glycosylation.

H. Someya, T. Itoh, S. Aoki

2626. Sequential glycosylation method using phenylthioglycoside with arming or disarming group in the aryl ring. **H. Dohi***, T. Kimura, T. Kanazawa, A. Ezawa, K. Kobayashi, R. Komai, Y. Nishida

2627. Synthesis of novel neogalacto-series glycosphingolipids from *Hirsutella rhossilienisis*. **i. ohtsuka***, T. Kanaya, n. hada, t. atsumi, T. Watanabe, n. kakiuchi

2628. Synthesis of fluorescent analogs of lipid-modified ganglioside GM3 for elucidating the function of ganglioside in the lipid raft.

A. Yamazaki, N. Komura, H. Ando*, A. Imamura, H. Ishida, M. Kiso

2629. Detailed examination of reactivity of mono-benzylated glucosyl and galactosyl donors. **A. Horii**, M. Konishi, A. Imamura, H. Ando*, H. Ishida, M. Kiso

2630. Automated electrochemical synthesis of TMG-chitotriomycin tetrasaccharide. **Y. Isoda**, T. Nokami*, N. Sasaki, S. Hayase, T. Itoh*, R. Hayashi, A. Shimizu, J. Yoshida*

2631. Reaction behavior of thioglycoside donors having aldehyde in leaving group.

R. Komai, H. Sakai, R. Sasaki, Y. Nishida, H. Dohi*

Hawaii Convention Center
Halls I, II, III

New Horizon of Process Chemistry by Scalable Reactions and Technologies (#426)

Organized by: K. Tomioka, R. Williams, R. Hwu, H. Sajiki, T. Shioiri, N. Yasuda
Presiding: K. Tomioka

Poster Session
19:00 – 21:00

2632. Alkylation of phenol with styrene over solid acid catalysts. Y. Hyeonjun, **H. Ahn***, Y. Lee, M. Jang, W. Kwak, S. Jung, M. Chung

2633. Isopropylation of benzene over modified zeolite with metal oxide to produce isopropylbenzene (Cumene).

M.C. Al-Kinany*

2634. Catalytic cracking of vacuum residue over modified zeolite to produce light olefins. **H.A. Almegren***, M.C. Al-Kinany, P. Edwards, T. Xiao

2635. Platinum group metal on carbon-catalyzed aqueous dehydrogenation of alcohols. **Y. Sawarna**, **S. Asai**, K. Morita, Y. Monguchi, H. Sajiki

2636. Liquid-phase mixture synthesis of 36 peptides using fluorous-Fmoc protection strategy and their ACE inhibitory activities. **N. Endo**, Y. Sugiyama, T. Hayashi, T. Shioiri, H. Hamamoto, M. Matsugi

2637. Palladium on spherical carbon (Pd/SC) as a catalyst for chemoselective hydrogenation. **H. Esaki***, T. Hattori, A. Tsubone, Y. Sawama, Y. Monguchi, K. Nosaka, K. Fukushima, H. Sajiki

2638. Chiral cyclopropane and cyclobutane forming-reactions using α -anion of nitriles: Asymmetric synthetic study of (1R,3R)-metofluthrin and (+)-grandisol.

T. Fujiwara, Y. Takahama, Y. Ashida, N. Matsuo, H. Nakatsuji, Y. Tanabe*

2639. Mill and environmentally friendly oxidative cleavage reaction of oxacyclic methanolos to lactones by 2-iodobenzamide catalyst-Ozone combination.

T. Fujiwara, Y. Horuchi, A. Yamada, H. Nambu, T. Yakura*

2640. Enzyme-catalyzed phenolic acetyl group manipulation technology-2: Application toward synthesis of glycosylated derivatives. **S. Hanamura**, R. Kobayashi, K. Asami, K. Hanaya, M. Shoji, T. Sugai*

2641. (E)-, (Z)-stereocomplementary parallel synthesis of (E)- and (Z)-tamoxifens.

Y. Ashida, **A. Honda**, Y. Sato, H. Nakatsuji, Y. Tanabe*

2642. Heterogeneous palladium catalyst supported on anion exchange resin for chemoselective hydrogenation and Suzuki–Miyaura reaction of chloroarenes.

T. Ichikawa*, M. Netsu, T. Hattori, T. Mizusaki, Y. Sawama, Y. Monguchi, H. Sajiki

2643. Regio- and stereoselective synthesis of (E)-1-bromo-2-iodoalkenes from internal alkynes. **M. Ide**, T. Iwasawa

2644. Regio- and stereoselective synthesis of vicinal (Z)-dihaloalkenyl silanes through *in situ* generated BrCl. **M. Ide**, T. Iwasawa

2645. Sn₂ displacement at the quaternary carbon center: A novel entry to the synthesis of α -D-substituted α -amino acids. **K. Ishihara**, H. Hamamoto, M. Matsugi, T. Shioiri

2646. Practical preparation of α -formyl esters from simple esters and methyl formate utilizing Ti-Claisen condensation and its utilization for useful building blocks. **S. Kajimoto**, Y. Ashida, H. Nakatsuji, Y. Tanabe

2647. Development of regioselective introduction of nucleophiles toward quinone monoacetals by design of specific acid catalyst. **T. Kamitanka**, N. Washimi, Y. Hu, T. Dohi, Y. Kita*

2648. Efficient hydroarylation of phenol with styrene employing mixed catalysts.

V. Kim, E. Shin*, M. Chung, W. Kwak

2649. Chiral phosphoric acid catalyzed asymmetric transfer hydrogenation of trifluoromethylated imines. **Y. Kiyo**, K. Saito, T. Akiyama*

2650. Enantioselective reaction of α -heteroacetonitriles using palladium pincer complexes with chiral bis(imidazoline)s.

M. Kondo, S. Nakamura, N. Kobayashi, T. Nishi

2651. Efficient synthesis of a PDE 4 inhibitor by using Pd–Cu catalyzed C–H/C–Br coupling of benzoxazole with a heteroaryl bromide. **K. Kuroda***, S. Tsuyumine, T. Kodama

2652. Green organic synthesis in gas-related multiphase reactions using micro- and nanobubbles strategy. **N. Mase***, Y. Nishina, K. Sato, T. Narumi, N. Watanabe

2653. FeCl₃-catalyzed self cleavage of methoxyphenylmethyl protected alcohols.

Y. Sawama*, **M. Masuda**, S. Asai, R. Goto, S. Nagata, S. Nishimura, Y. Monguchi, H. Sajiki

2654. Development of standard solutions for qNMR. **T. Miura**, S. Nakao, S. Takaoka, Y. Yamada*

2655. One-pot N-arylindole synthesis from 2-bromophenethylamine. **Y. Monguchi***, T. Marumoto, H. Takamatsu, Y. Sawama, H. Sajiki

2656. Chiral phosphoric acid catalyzed asymmetric synthesis of dihydroquinolinoles using aza-Michael reaction.

Y. Moriya, K. Saito, T. Akiyama*

2657. Synthesis of procyanidins and their derivatives using silyl-protecting group.

N. Nakajima*, M. Hamada, T. Kishimoto, A. Saito

2658. Development of magnetic nanoparticle-supported iodoarene oxidative catalysts and its application.

H. Nambu, I. Shimokawa, T. Fujiwara, T. Yakura*

2659. Concise synthesis of all stereoisomers of dendramide A employing fluorous-Fmoc reagents.

K. Oguri, N. Endo, Y. Sugiyama, H. Hamamoto, T. Shioiri, M. Matsugi

2660. Stainless steel-mediated hydrogen generation from water using ball milling and its application.

Y. Sawama, M. Niikawa, T. Kawajiri, R. Goto, Y. Monguchi, H. Sajiki

2661. Study on the synthesis of styrenated phenol using organometallic catalysts.

S. Son, J. Kim, H. Ahn, M. Jang, W. Kwak, S. Jung, M. Chung*

2662. Asymmetric epoxidation of aromatic olefins using light fluorous salen manganese complex: Enhancement of enantioselectivity by the addition of benzonitrile as a cosolvent.

Y. Sugiyama*, Y. Kobayashi, H. Miyazaki, H. Hamamoto, T. Shioiri, M. Matsugi

2663. Platinum group metal on carbon-catalyzed multiple deuteration of arenes and alkanes in 2-propanol/D₂O mixed solvent.

T. Yamada, Y. Monguchi, Y. Sawama, H. Sajiki

2664. Enzyme-catalyzed phenolic acetyl group manipulation technology-1: Application to the synthesis of physiologically active natural products.

K. Yashiro, S. Mandal, K. Hanaya, M. Shoji, T. Sugai*

Hawaii Convention Center Halls I, II, III

Asymmetric Supramolecular Catalysis (#451)

Organized by: J. Takacs, S. Moteki, J. Green

Poster Session
19:00 – 21:00

2665. Development of self-assembled asymmetric catalyst based on two-point hydrogen bonding interaction.

T. SHISHIDO, M. Yamanaka*

2666. Synthesis of structurally-chiral molecules aiming for the dynamic conformational switching.

S. Handa, H. Goto, H. Sugimoto*

2667. Ligand-enabled multiple absolute stereocontrol in palladium-catalyzed [3 + 2] cycloaddition.

N. Imagawa, K. Ohmatsu, T. Ooi*

2668. Selective O-acylation of *meso*-1,2-diol with a rotaxane organocatalyst.

T. Iwase*, K. XU, K. Nakazono, T. Takata

* Principle Author

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TECHNICAL PROGRAM

Hawaii Convention Center
Halls I, II, III

Synthetic Modulators of Protein-Protein Interactions (#461)

Organized by: P. Arora, D. Fairlie,
A. Kennan, K. Kumar, S. Sidhu, ,
Presiding: P. Arora

Poster Session
19:00 – 21:00

2669. γ-Turn peptidomimetic scaffold and its application: From scaffold-hopping to synthesis. **J. Hah**, M. Kim, C. Lee

2670. Inhibitors of the pore-forming protein perforin as potential immunosuppressive agents. **J. Spicer***, C. Miller,
P. O'Connor, J. Jose, J. Jaiswal,
S. Jamieson, W. Denny, R. Law,
J. Whistock, H. Akhlaghi, J. Trapani

2671. Structural development of stapled short helical peptides as vitamin D receptor (VDR) coactivator interaction inhibitors. **T. Misawa***, Y. Demizu, M. Kurihara

2672. Pharmacological chaperones targeting cancer-associated MCL-1 and Parkinson's disease-associated α-synuclein. **M. Oh**, J. Lee, Q. Hoang, H. Lim*

2673. Novel BRD4 inhibitors with a N6-benzoyladenine skeleton. **T. Noguchi-Yachide***, T. Sakai,
Y. Hashimoto, T. Yamaguchi

2674. Development of transrepression-selective liver X receptor (LXR) ligands. **S. Nomura**, K. Endo-Umeda, A. Aoyama,
M. Ishikawa*, M. Makishima,
Y. Hashimoto

2675. Discovery and synthesis of a novel non-covalent inhibitor for protein-protein interaction between Nrf2 and Keap1. **D. Yasuda**, T. Ohe, R. Obata,
K. Takahashi, T. Mashino, M. Komatsu,
Y. Ichimura, M. Yamamoto, R. Imamura,
H. Kojima, T. Okabe, T. Nagano*

2676. Novel peptidomimetic compounds as anticancer agents and their molecular docking studies. **J. Lee***, H. Lee

2677. Novel tools to structurally characterize protein-protein interactions. **R. Oliva**,
E. Chermak, L. Cavallo

2678. Polymorphological profiles of phenanthridinone derivatives. **Y. Nishiyama**, T. Misawa, H. Aoyama,
S. Fujii, M. Ishikawa, Y. Hashimoto

Sunday Morning

Hilton Hawaiian Village
Rainbow Tower, Rainbow 3

Anion Receptors (#31)

Organized by: B. Hay, F. Pfeffer, B. Wu,
C. Jia, R. Custelcean
Presiding: A. Flood, B. Wu

8:00 – 2679. New anion receptors and transporters. **P. Gale***

8:30 – 2680. Understanding and application of anion-π interactions. **D. Wang**

9:00 – 2681. Discriminating anions through tunable electronic interactions. **S. Saha***

9:30 – 2682. Ion-pairing assemblies based on anion-responsive π-electronic molecules. **H. Maeda***

10:00 Break

10:15 – 2683. Luminescent lanthanide(III) complexes for anion recognition. **M. Albrecht***

10:45 – 2684. Interactions of anions with halogen and chalcogen bond donors. **M.S. Taylor***

11:15 – 2685. Tripodal receptors for anion binding and sensing. **P. Anzenbacher***

Hilton Hawaiian Village
Mid-Pacific Center, South Pacific Ballrm 1

New Green Techniques for Medicinal Chemistry (#148)

Organized by: W. Zhang, I. Ryu, P. Toy
Presiding: I. Ryu, M.P. Sibi

8:00 – 2686. Development of a "green strategy" within medicinal chemistry at Genentech and in the pharma industry. **M. Bryan**

8:30 – 2687. Green chemistry at Merck: Green by Design through innovation. **J. Yin***

9:00 – 2688. Nanomole-scale high-throughput chemistry - a green approach to the synthesis of medicinally relevant molecules. **T. Cernak***, A. Buitrago Santanilla,
S. Dreher*, E.L. Regalado, P. Vachal,
L. Campeau, I. Davies, C. Welch

9:20 – 2689. Chemosynthetic livers: Predict, prepare, and prove the structure, activity, and toxicity of drug metabolites. **M.S. Chorghade***, R.S. Chorghade

9:40 – 2690. Free-radical-based site-selective C-H to C-C conversion. **I. Ryu***

10:10 – 2691. New synthetic reactions of N-heterocyclic carbene boranes. **D.P. Curran***

10:40 – 2692. Development of green conversions of biomass in hydrophobic ionic liquids. **A. Kamimura**

11:10 – 2693. Synthesis of novel polymers from biomass and their programmed degradation. **M.P. Sibi***, E. Serum,
C. Sutton, R. Raghunathan, R. Krishnan,
S. Jayaraman*, D. Webster,
R. Saravananumar

11:40 – 2694. Lignin disassembly and the role of paired-electrolytes in the sustainable synthesis of new synthetic building blocks. **B. Nguyen, M. Llorente,
C.P. Kubik, K.D. Moeller**

Hilton Hawaiian Village
Mid-Pacific Center, Coral 2

Applications of C-H Functionalization (#169)

Organized by: P. Vachal, Z. Shi, C. Li,
H. Davies, K. Itami, H. Lebel

8:00 – 2695. C-H arylation in combination with decarboxylative cross-couplings as a modular route to biologically important thiophene-based targets. **P. Forgione**

8:30 – 2696. Design of axially chiral phenanthrolidine ligands for enantioselective C-H functionalization. **Y. Naganawa***,
H. Nishiyama*

8:50 – 2697. Development of metal-catalyzed reactions to access N-heterocycles from nitroarenes. **T. Driver**

9:20 – 2698. Branch selective Ir-catalyzed hydroarylation of monosubstituted alkynes via a cooperative destabilization strategy. **G.E. Crisenzia***, J. Bower

9:40 – 2699. Adventures in aldehyde C-H bond activation. **V.M. Dong***

10:10 – 2700. Stereoselective radical C-H amination by Co(II)-based metalloradical catalysis. **P. Zhang***

10:40 – 2701. Palladium(0)-catalyzed C(sp³)-H bond activation as a strategy for the construction of polycyclic systems. **O. Baudoin***

11:10 – 2702. Nickel(II)-catalyzed oxidative coupling between C(sp³)–H bonds in benzamides and C(sp³)–H bonds in toluene derivatives. **Y. Aihara**, N. Chatani*

11:30 – 2703. Catalytic aerobic platform for the selective functionalization of phenolic C-H bonds. **Z. Huang, K. Esguerra,
J. Lum***

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 1

Strategies and Tactics for Complex Molecule Synthesis (#174)

Organized by: C. Forsyth, C. Lee,
L. Barriault, J. Cha
Presiding: C. Lee, B. Wang

8:00 introduction

8:05 – 2704. Radical-based approach for synthesis of complex natural products. **M. Inoue***

8:35 – 2705. Total synthesis of natural products containing multisubstituted arenes via a 6π electrocyclization/aromatization strategy. **A. Li**

9:05 – 2706. Streamlined syntheses of complex tetracyclic diterpenoids. **X. Lei***

9:35 break

9:40 – 2707. Total synthesis of ustiloxin D. **C.A. Hutton***, A.L. Brown

9:55 – 2708. Protecting group free strategy for the sustainable synthesis of polyketide natural products. **R.S. Chapman***, P. Plucinski, M. Jones,
S.D. Bull

10:10 – 2709. Nanomole-scale high-throughput chemistry for the synthesis of complex molecules. **L. Campeau**

10:25 – 2710. Colorful azulene-based protecting group for carboxylic acids, alcohols, and amines. **T.W. Bevan***,
H.J. Wong, P.T. Northcote, J.E. Harvey

10:40 – 2711. Recent innovations in alkyne chemistry. **G.B. Dudley***

10:55 Break

11:00 – 2712. Relative and absolute configurations of Phaeosphaeride A: Total synthesis of ent-Phaeosphaeride A. **K. Kobayashi***, M. Nakamura,
Y. Kobayashi, O. Tamura, H. Kogen*

11:20 – 2713. Highly convergent, enantioselective, and conceptually novel synthesis of polydeoxypropionate. **S. Xu**, A. Oda,
T. Bobinski, H. Li, E. Negishi*

11:40 – 2714. Lipase-catalyzed asymmetric synthesis of multifused optically active cyclic molecules by one-pot sequential dynamic kinetic resolution/intramolecular Diels-Alder reaction. **K. Sugiyama**,
S. Kawanishi, Y. Oki, M. Kamiya, M. Egi,
S. Akai*

12:00 closing remarks

Hilton Hawaiian Village
Mid-Pacific Center, Sea Pearl Suites 1 & 2

Cooperative Cocatalysis with Two Different Metals (#270)

Organized by: S. Blum, Y. Nakao,
S. Chang

8:00 – 2715. Acceptorless dehydrogenation of alkanes through cooperative base metal catalysis . **J.G. West**,
E.J. Sorensen*

8:30 – 2716. Multimetallic cross-electrophile coupling reactions and design principles. **D.J. Weix***

9:10 Break

9:20 – 2717. Enabling multiple catalytic transformations from a single heterobimetallic design strategy. **N.P. Mankad**

10:00 – 2718. Synergistic divergent dipolar cycloaddition reaction from non-dipolar compounds using dual catalysis system. **H. Jeon, S. Lee***

10:30 – 2719. Recent progress in cooperative asymmetric catalysis. **M. Shibasaki**

Hilton Hawaiian Village
Tapa Tower, Tapa Ballrm 2

Chemical Glycosylation: Methods and Mechanisms (#306)

Organized by: T. Lowary, X. Huang,
S. Hung, K. Tanaka
Presiding: K. Tanaka

8:00 – 2720. Scalable and stereoselective synthesis of 1,2-cis-2-amino sugars via nickel catalysis. **H.M. Nguyen**

8:30 – 2721. General strategy for stereospecific synthesis of rare higher carbon sugars and its application thereof. **K.T. Mong***

9:00 – 2722. Examination of 1,2-trans-selective glycosidation of glycosyl donors bearing 2,3-cyclic protecting group. **N. Yagami**, M. Konishi, H. Tamai,
A. Ueki, A. Immura, H. Ando*, H. Ishida,
M. Kiso

9:15 – 2723. Synthesis of C-2 functionalized liduronic acid derivatives. **S. Mohamed***

9:30 – 2724. Study on stereoselective cis-glycosylations through NAP ether-mediated intramolecular aglycon delivery. **A. Ishiwata***, Y. Ito

9:45 – 2725. Mechanistic insights into the gold(I)-catalyzed glycosylation with glycosyl ortho-alkynylbenzoates as donors. **B. Yu**

10:15 Break

10:25 – 2726. De novo synthesis of carbohydrate for medicinal chemistry. **G.A. Odoherty**

10:55 – 2727. Glycosylation of 2,4-O-(o-xylylene)-bound thioglucoside. **Y. Sakamoto***, Y. Ito*

11:10 – 2728. Novel chemical glycosylation with recognition of alcohol chirality and its application to natural product synthesis. **T. Kimura**, D. Takahashi, K. Toshima*

11:25 – 2729. Catalytic stereoselective synthesis of glycosides. **M. Galan***

Hilton Hawaiian Village
Mid-Pacific Center, Nautilus 1

Synthetic Modulators of Protein-Protein Interactions (#461)

Organized by: P. Arora, D. Fairlie,
A. Kennan, K. Kumar, S. Sidhu, ,
Presiding: A. Kennan

8:00 Break

8:30 Opening Remarks

8:35 – 2730. Protein domain mimetics as modulators of protein-protein interactions. **P. Arora***

9:00 – 2731. Simulating secondary structure: β-strand/sheet peptidomimetics. **S. Thompson**, P.C. Kripe, J.E. Ross,
J.T. Han, A.D. Hamilton

9:20 – 2732. Small-molecule mimic for the side chains of hydrophobic α-helical hot spots and its application to the β-Catenin/B-cell lymphoma 9 protein-protein interaction. **H. Ji***

9:40 Break

9:50 – 2733. Inhibition of helix mediated protein-protein interactions using designed molecules. **A.J. Wilson**

10:15 – 2734. A-peptides and their derivatives for protein surface recognition. **J. Cai***

10:35 – 2735. Covalent control of peptide loop structure. **J. Kritzer***

10:55 Break

11:05 – 2736. Allosteric modulation of conformationally dynamic transcription factor complexes. **A.K. Mapp***

11:30 – 2737. Bioreversible protein modifications that engender cellular delivery. **R.T. Raines***

PHYS

Area 5 – Physical, Theoretical, & Computational

Tuesday Morning

Hawaii Convention Center
308A

Ultrafast Intense Laser Chemistry (#35)

Organized by: K. Yamanouchi, R. Lewis,
F. Legare, Q. Gong
Presiding: Q. Gong

8:00 Opening Remarks

8:05 – 1. Coherent control at its most fundamental. M. Sayler, T. Rathje, M. Möller,
P. Wustelt, G.G. Paulus*

8:30 – 2. Strong-field coherent control: Unpacking the role of phase. D.B. Foote,
Y. Lin, W.T. Hill*

* Principle Author

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8:55 – 3. Adiabatic ionization creates a “pure” wave packet in the strong field regime for control at a conical intersection in acetophenone derivatives. **R.J. Lewis***

9:20 – 4. Synergy of chirped and multipulse excitation: Control of population and vibrational coherence using. E. Brühl, I. Afa, C. Serrat, T. Buckup, **M. Motzkus***

9:45 Break

10:00 – 5. Intense IR laser induced electron rescattering study on hydrocarbon molecules. **Y. Ito**, M. Okunishi, W. Chuncheng, R.R. Lucchese, T. Morishita, O.I. Tolstikhin, L.B. Madsen, K. Ueda*

10:10 – 6. Laser-assisted electron scattering by light-dressed Xe atoms in a femtosecond intense laser field. Y. Morimoto, **R. Kanya**, K. Yamanouchi*

10:35 – 7. Development of a femtosecond laser-assisted electron scattering apparatus equipped with an angular-resolved time-of-flight analyzer. **K. Ishida**, R. Kanya, K. Yamanouchi*

10:45 – 8. Development of trapped ion electron diffraction apparatus for determination of geometrical structure of molecular ions. **H. Tanaka**, K. Kato, R. Kanya, K. Yamanouchi*

10:55 – 9. Intense laser-induced population inversion of N_2^+ . **H. Xu***, E.V. Lotstedt, K. Yamanouchi

Hawaii Convention Center
301A

Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60)

Organized by: A. Kovalenko, B. Pettitt, F. Hirata
Presiding: F. Hirata, A. Kovalenko

8:00 – 10. Comparing theory, heuristics, and simulations in solution. K. Dyer, J. Perkyns, D. Karandur, C. Zhang, **M. Pettitt***

8:30 – 11. Hydrophobic interaction: From statics to kinetics. **A. Lazar**

9:00 – 12. Approaching quantitative accuracy with integral equation-based solvation models. **S.M. Kast***

9:30 – 13. Mechanism of one-to-many molecular recognition accompanying target-dependent structure formation: For the tumor suppressor p53 protein. **T. Hayashi**, H. Oshima, S. Yasuda, M. Kinoshita

9:45 – 14. Multiscale simulation of fullerene solvation and aggregation behaviors in organic solvent. **C. Wang**, C. Hua*

10:00 Coffee Break

10:15 – 15. Aqueous solutions: New insights from large-scale computer simulations. R. Gupta, **G. Patey***

10:45 – 16. Fluctuation-aggregation duality in complex liquids. **A. PERERA***

11:15 – 17. Free-energy calculation with the method of energy representation with application to the binding of small molecules into polymers. **N. Matubayasi***

11:45 – 18. Systematic method to estimate solvation free energies from 2PT molecular dynamics. **H. Lee***, H. Lim, H. Kim

Hawaii Convention Center
308B

New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems (#84)

Organized by: T. Carrington, J. Bowman, D. Zhang
Presiding: E.L. Sibert

8:00 Opening Remarks

8:05 – 19. Calculation of vibrational ground and excited states of malonaldehyde and their tunneling splittings. **H. Meyer***, M. Schröder

8:35 – 20. CO₂ inside the clathrate hydrate cavities: A quantum dynamic study for comparing with experiments. **D.J. Arismendi Arrieta**, Á. Valdés, R. Prosmitsi

8:55 – 21. Symmetrical quasi-classical model for classical molecular dynamics simulations of electronically non-adiabatic processes. **W.H. Miller**

9:25 – 22. Efficient calculation of anharmonic vibrational spectra using localized modes. P.T. Panek, **C.R. Jacob**

9:45 Break

10:00 – 23. Understanding and controlling chemical reactions: Applications of the multiconfiguration time-dependent Hartree method. **F. Gatti**, H. Meyer, B. lasorne, S. Guérin, R. Marquardt

10:30 – 24. Size-consistent multipartitioning QM/MM: A stable and efficient adaptive QM/MM method. **H.C. Watanabe***, T. Kubar, M. Banro, M. Elstner, M. Sakurai

10:50 – 25. Multidimensional quantum dynamics with and without a potential energy surface: Parameterized bases and anharmonic spectra in up to 15D. **S. Manzhos***, T. Carrington, R. Dawes, X. Wang, H. Guo

11:20 – 26. Variational multiconfigurational quantum dynamics using moving Gaussian basis sets: Flexible frozen Gaussian-based hierarchical representations. **I. Burghardt**, P. Eisenbrandt, M. Ruckenbauer, S. Römer

Hawaii Convention Center
305B

Deciphering Molecular Complexity from Single Molecules to Cellular Networks (#121)

Organized by: T. Komatsuzaki, J. Wang, J. Wu
Presiding: T. Komatsuzaki, J. Wu

8:00 Opening Remarks

8:05 – 27. Finding the macro-micro boundary. **R. Berry**

8:40 – 28. Multiscale method for dynamics simulations of biomolecular systems. **R. Luo***

9:10 – 29. Complex folding transition of the B domain of protein A investigated by the high-speed measurement of single-molecule FRET time series. H. Okawa, K. Kamagata, M. Arai, **S. Takahashi***

9:40 Break

9:55 – 30. Robustness of rotary catalysis of F1-ATPase rotary motor tested by creating an artificial rotary motor molecule. **H. Noji***

10:30 – 31. Conformational fluctuations in DNAs and enzymes. **J. Cao***

11:00 – 32. Single-molecule method for counting ligands associated with a conformational transition: Linking ion uptake to nucleic acid folding. **D.R. Jacobson***, O.A. Saleh

Hawaii Convention Center
305A

Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130)

Organized by: A. Wilson, P. Schwerdtfeger, K. Kim, Z. Lin, T. Cundari
Presiding: A. Wilson

8:00 Introductory Remarks

8:05 – 33. Computational insight into nickel-catalyzed carbon–carbon vs. carbon–boron coupling reactions of primary, secondary, and tertiary alkyl bromides. M. Cheung, F. Sheong, T. Marder, **Z. Lin**

8:35 – 34. Transition metals in astrochemistry: Which roads lead to a better understanding of astrobiology?. **N.J. DeYonker***, T.N. Brown, K.O. Brown

9:05 – 35. Automated exploration of adiabatic and nonadiabatic channels in organometallic complexes. **S. Maeda***, Y. Harabuchi, M. Gao, G. Zeng, T. Taketsugu

9:35 BREAK

9:35 BREAK

9:50 – 36. Ground and excited states of the $[Fe(H_2O)_6]^{2+}$ and $[Fe(H_2O)_6]^{3+}$ clusters: Insight into the electronic structure of the $[Fe(H_2O)_6]^{2+}$ – $[Fe(H_2O)_6]^{3+}$ complex. **S.S. Xantheas***, E. Millordos

10:20 – 37. N₂O activation by a vanadium(III) complex. **B.F. Yates***, R. Robinson, M.F. Shaw, R. Stranger

10:50 – 38. Reduction of chromium oxide by methane: Density functional theory studies. **K.M. Skjelbred***, P. Åstrand, S. Andersson, J.A. Stenveng

11:10 – 39. Activation of CH₄ by Th⁺ as studied by guided ion beam mass spectrometry and quantum chemistry. **P.B. Armentrout**, R.M. Cox, W.A. de Jong

Hawaii Convention Center
306B

Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134)

Organized by: P. Piotrowiak, M. Fujii, J. Tang, B. Zhang
Presiding: P. Piotrowiak, B. Zhang

8:00 Opening Remarks

8:05 – 40. Mapping atomic motions with ultrabright electrons: The chemists' Gedanken experiment enters the lab frame. **R. Miller***

8:45 – 41. Quantized chromatic aberrations and temporal resolutions in ultrafast electron microscopy. **D.J. Flannigan***, D.A. Plemmons, D.R. Cremons, D.T. Valley

9:15 – 42. Imaging ultrafast molecular reactions with free electron laser radiations. **Y. Jiang**

9:45 – 43. Nonadiabatic dynamics in polyatomic molecules by femtosecond time-resolved photoelectron imaging. **B. Zhang***

10:15 Break

10:30 – 44. Picosecond photobiology: Watching a signaling protein function in real time via 150-picosecond time-resolved X-ray diffraction and solution scattering. **P. Anfinrud***, F. Schotte, H. Cho, J. Kyndt, H. Kamikubo, M. Kataoka

11:00 – 45. Femtosecond time-resolved impulsive stimulated Raman study of the primary process of photoactive yellow protein. H. Kuramochi, S. Takeuchi, K. Yonezawa, H. Kamikubo, M. Kataoka, **T. Tahara**

11:30 – 46. Observation of molecular orientation of human hair α-keratin fibers by a VSFG detected IR super-resolution microscopy. **M. Sakai***, K. Ushio, Y. Watase, M. Fujii

Hawaii Convention Center
313C

Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)

Organized by: J. Hasegawa, M. Collins, M. Gordon, P. Piecuch, T. Taketsugu
Presiding: P. Piecuch

8:00 Opening address

8:10 – 47. Recent progress in density functional theory. **D.G. Truhlar***

8:40 – 48. Electronic excitations from pairing matrix fluctuation and particle-particle random phase approximation. **W. Yang**

9:00 – 49. Assignments of ground and excited states of 3D carbon and boron clusters from P3+ and NR2 electron-propagator theory. **J.V. Ortiz***

9:20 – 50. Does CC2 and CC3 theory offer quality potential surfaces for excited electronic states?. **J.F. Stanton***

9:50 – 51. Metastable electronic states and complex variable approaches: A fresh look at the old challenge. **A. Krylov**

10:20 – 52. Solvent effects in excited states: PCM SAC-Cl study. **M. Ehara**, R. Fukuda

10:50 – 53. Development of linear-scaling excited-state calculations: Divide-and-conquer approaches. **H. Nakai**

11:20 – 54. Excited states in condensed matter from embedded correlated wavefunction theory. **E.A. Carter***

Hawaii Convention Center
313A

Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168)

Organized by: A. Terasaki, S. Anderson, N. Gaston
Presiding: S.L. Anderson

8:00 Opening address

8:05 – 55. Super- and hyper halogens-A class of superatoms. **P. Jena**

8:35 – 56. Nanocluster superatom formation using ion sources based on high-power impulse magnetron sputtering. **A. Nakajima***

9:05 – 57. Determining the structure of transition metal clusters and their derivatives by trapped ion electron diffraction. **M. Kappes***, D. Schooss

9:25 – 58. Uncovering structure-property relationships: From studies of pure and supported metal clusters and colloids to their use in catalysis and sensing. **V. Golovko***, D. Anderson, R. Adnan, B. Donoeva, D. Ovoshchikov, J. Ruzicka, D. Padayachee, A. Marshall, G. Andersson, G.F. Metha, W. Włodarski

9:45 break

10:00 – 59. Doped metal clusters on oxides: Rationalization and design through the prism of chemical bonding. **A. Alexandrova***

10:30 – 60. Molecular silver nNanoparticles: Chemical, optical, and structural principles. **T.P. Bigioni***

11:00 – 61. Molecular simulation of Ag nanoparticle nucleation from solution: Redox-reactions direct the evolution of shape and structure. **D. Zahn***, T. Milek

11:20 – 62. Toward the creation of stable, functionalized metal clusters. **Y. Negishi***

Hawaii Convention Center
304A

Theory of Main Group Chemistry Beyond First Row (#183)

Organized by: T. Dunning, M. Gordon, P. Schwerdtfeger, C. Choi
Presiding: T. Dunning

8:00 – 63. Recoupled pair bonding: Insight into chemistry beyond the first row and beyond Earth. **D.E. Woon**

8:30 – 64. Bonding analysis using the atomic orbitals found within molecular wavefunctions. **M.W. Schmidt**

9:00 – 65. Bonding energetics of main group compounds. **D.A. Dixon***

9:30 – 66. Non-covalent interactions beyond the first row: Big challenges from small π-type dimers. **G.S. Tschumper**

10:00 – 67. Experimental and theoretical investigations on the elementary reactions of F₂ with organosulfur molecules. **J. Lin***

10:30 – 68. Structure, bonding, and energetics of lower p-block species: Developments and applications. **A. Wilson***

11:00 – 69. Chemical bonding in diatomic molecules of the first and higher octal rows of the periodic system. **G. Frenking***

* Principle Author

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11:30 – 70. Expanding the Bent's rule toward main group elements: Hybridization trends across the periodic table.
I. Alabugin, S. Bresch

Hawaii Convention Center
304B

Latest Development of Advanced Vibrational Spectroscopy (#187)

Organized by: K. Iwata, S. Asher, D. Phillips, Y. Furukawa
Presiding: Y. Furukawa, K.C. Gordon

8:00 – 71. Femtosecond stimulated Raman spectroscopy: A vibrationally specific probe of reactive nonadiabatic coupling.
R.A. Mathies

8:25 – 72. Development of stimulated Raman scattering interferometer and its application to the chemical contrasted imaging of buried layers and interfaces.
M. Banno, T. Kondo, H. Yu*

8:45 – 73. Self-localized excitations formed in π -conjugated polymers in solution: Femtosecond near-IR absorption and stimulated Raman studies.
T. Takaya, M. Shinohara, K. Iwata*

9:00 – 74. Photoinduced structural change of aromatic oligomers in water observed by ultrafast spectroscopy.
M. Iwamura*, R. Wakabayashi, J. Maeba, K. Nozaki, S. Takeuchi, T. Tahara

9:20 – 75. Excited-state intramolecular proton transfer investigated by femtosecond electronic and vibrational spectroscopy.
Y. Pang*, M. Jen, S. Lee, T. Jang

9:35 – 76. Theoretical-computational modeling of excited state proton transfer reactions through multiresolution vibrational analysis.
G. Donati*, A. Petrone, P. Cimino, N. Rega*

9:55 break

10:05 – 77. Application of Raman spectroscopy to organic electronic devices.
Y. Furukawa

10:30 – 78. Measurements and analyses of the infrared and Raman spectra of radical cation of [34](1,2,4,5)cyclophane: Observation of electron-molecular vibration interaction by infrared spectroscopy and large amplitude bridged ring vibrations by near-infrared resonance Raman spectroscopy.
A. Sakamoto*, H. Okajima, N. Tanaka, T. Shimmyozu

10:55 – 79. Probing the entire vibrational frequency range with continuum mid-IR laser pulses.
A.M. Stigle, H. Vanselous, P.B. Petersen

11:15 – 80. Single-mode interband cascade lasers for spectroscopic applications.
L. Hildebrandt*, J. Scheuermann, M. Edlinger, R. Weih, L. Nähle, M. Fischer, J. Koeth, M. Kamp, S. Höfling

11:30 – 81. Raman spectroscopic observation of collisional reaction between H_2SO_4 and NaOH droplets.
K. Anahara*, J. Kohno

11:45 – 82. In situ variable temperature infrared spectroscopy of the vitrification process: New molecular insights on an intriguing phenomenon.
A. Laventure, A. Soldera, O. Lebel, C. Pellerin*

Hawaii Convention Center
301B

Frontier Chemical Applications Using Accelerator Based Photon Sources (#414)

Organized by: K. Asakura, T. Sham, L. Chen
Presiding: L.X. Chen

8:00 Welcome coffee
8:20 Welcome message
8:30 – 83. Ultra slow Muon microscopy - a new method to study function across interfaces in materials and life science.
E. Torikai, Y. Miyake, R. Kadono, M. Iwasaki

9:00 – 84. Total-reflection high-energy positron diffraction (TRHEPD): A novel method for the analysis of the surface atomic arrangements.
T. Hyodo*, I. Mochizuki, K. Wada, Y. Fukaya, M. Maekawa, A. Kawasuso, T. Shidara, A. Ichimiya, H. Ariga, K. Asakura

9:20 – 85. Neutron analysis of cytochrome c using the maximum entropy method (MEM).
Y. Sugawara*, S. Yamamura, K. Kusaka, T. Yamada

9:40 – 86. Synchrotron X-ray absorption spectroscopy study of nanomaterials for energy applications.
X.J. Sun*

10:00 break

10:20 – 87. In-situ structural characterization of interfacial homogeneous and amorphous metal oxide catalysts using X-ray scattering and pair distribution function analyses.
G. Kwon*, J.D. Emery, J. Thomsen, G. Brudvig, R. Crabtree, A.B. Martinson, D.M. Tiede*

10:50 – 88. Measurement of carbon condensates using small-angle X-ray scattering during detonation of the explosive hexanitrostilbene.
T.M. Willey*, M. Bagge-Hansen, L. Lauderbach, R. Hodgin, S. Bastea, L. Fried, C. May, T. Gruber, B. Jensen, J. Ilavsky

11:10 – 89. Tracking drug loading and unloading processes involving calcium silicate hydrate carrier and ibuprofen (IBU): An X-ray absorption spectroscopy study.
T.K. Sham*, X. Guo, Z. Wang, J. Wu, Y. Hu, J. Wang, Y. Zhu

Hawaii Convention Center
306A

Frontiers of Photon Upconversion Based on Triplet-triplet Annihilation (#420)

Organized by: P. Zhang, Y. Murakami, J. Zhao
Presiding: Y. Murakami, P. Zhang, J. Zhao

8:00 Opening remark

8:05 – 90. Unusual solar photoconversion: Sensitized triplet fusion.
F.N. Castellano

8:35 – 91. Photochemical upconversion for solar energy.
T. Schmidt

9:05 – 92. Experimental sunlight engineering, based on energy transport in dense populated organic triplet ensembles.
S. Baluschev*, K. Landfester

9:35 Break

9:50 – 93. Triplet-triplet annihilation upconversion in the aqueous and dry phases: Challenges, solutions, and more problems.
J. Kim*

10:20 – 94. TTA between and within dendritic macromolecules.
S. Vinogradov*

10:50 – 95. Low-power photon upconversion through triplet-triplet annihilation in polymeric materials.
C. Weder*

11:20 – 96. Effect of solvent viscosity on TTA-based photon upconversion: Studies in ionic liquids.
Y. Murakami*, T. Ito, A. Kawai

Hawaii Convention Center
313B

Computational Modeling of Magnetic Materials and Magnetic Properties (#423)

Organized by: J. Peralta, A. Soncini, T. Nakajima
Presiding: J. Peralta, A. Soncini

8:00 – 97. Ab initio study of magnetization blocking in strongly anisotropic magnetic complexes.
L. Chibotaru

8:30 – 98. Magnetic ordered structure dependence of magnetocaloric effect.
R. Tamura, S. Tanaka, T. Ohno, H. Kitazawa

8:40 – 99. Calculating magnetic properties of heavy-element compounds.
J. Autschbach

9:10 – 100. Demagnetisation effects in dipolar systems.
M. Twengstrom*, L. Bovo*, M. Gingras, S. Bramwell, P. Henelius

9:20 – 101. Density-functional theory in magnetic fields.
T. Helgaker*, A. Borgoo, U. Ekström, J. Furness, J. Gauss, S. Kvaal, K. Lange, S. Reimann, S. Stopkowicz, A. Teale, E. Tellgren, J. Verbeke

9:50 Coffee Break

10:10 – 102. Single-molecule magnets and related molecules: Structural, magnetic, and quantum properties.
G. Christou

10:40 – 103. Electronic structure of molecular magnetic systems: Successes within GGA and challenges for SiC.
M.R. Pederson*

11:10 – 104. Tailoring electronic and magnetic properties of MoS₂ nanotubes.
G. Lee, N. Li*

11:20 – 105. Theoretical investigation of magnetic exchange interactions in dilute magnetic semiconductor quantum dots induced by defects.
J. Goings*, X. Li

Hawaii Convention Center
310 Theatre

Frontiers of Plasmon Enhanced Spectroscopy (#428)

Organized by: Y. Ozaki, Z. Tian, B. Ren, N. Halas, A. Brolo, T. Itoh, M. Moskovits
Presiding: N. Halas, Y. Ozaki

8:00 opening

8:05 – 106. Recent developments in tip-enhanced Raman spectroscopy.
R.P. Van Duyne*

8:35 – 107. Aluminum plasmonics for surface-enhanced spectroscopies.
N. Halas*

9:05 – 108. Coherent plasmons in surface enhanced spectroscopies.
P. Nordlander*

9:25 – 109. Plasmon on single nanoparticles for sensing the reactions.
Y. Long*

9:45 – 110. Raman activity and dynamics of plasmons studied by ultrafast scanning near-field optical microscopy.
K. Imura*, K. Imaeda

10:05 Break

10:20 – 111. Subnanometric plasmonics: Confining light to atomic-scale dimensions.
J. Aizpurua*, M. Barby, P. Koval, F. Marchesin, R. Esteban, A.G. Borisov, D. Sanchez-Portal

10:40 – 112. Plasmonic dimers and trimers: On the role of gap size and symmetry.
G. Haran*, L. Chuntonov, N. Zohar

11:00 – 113. Tuning of the surface plasmon resonance in the UV-IR range for wider applications.
K. Okamoto, K. TAMADA

11:15 – 114. Plasmonic spectroscopy: What determines the plasmonic band intensity, its shift in a dielectric medium, or on a substrate of high dielectric function?
N. Hooshmand*, J.A. Bordley, M.A. El-Sayed

11:30 – 115. Plasmonic-coupling-based enhanced performance in surface plasmon resonance spectroscopy.
D. Kim*, K. Chung, J. Lee, J. Choi, Y. Jang

11:45 – 116. When the signal is from the original molecule detected: Surface-enhanced Raman scattering measurement of 4-aminobenzenethiol at single-molecule level.
Y.S. Yamamoto*, Y. Kayano, T. Itoh, S. Nakanishi

Hawaii Convention Center
307AB

Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)

Organized by: H. Sekiya, T. Zwier, M. Fujii, E. Bieske, N. Kim
Presiding: N. Kim, H. Sekiya

8:00 Opening Remarks

8:05 – 117. Temperature dependence of hydrogen bond network structures probed by infrared spectroscopy of gas phase clusters.
A. Fujii*

8:30 – 118. Understanding inter- and intramolecular factors affecting red-shifts for the proton stretch vibrational frequency in hydrogen-bonded complexes.
D. Pines, P.M. Kiefer, J.T. Hynes, E. Pines*

8:50 – 119. Hydrogen-bonding interactions of uric acid complexes with water/ melamine identified by near- and mid-IR spectroscopy.
H. Saigusa

9:15 – 120. What can we learn on hydroxide solvation from theoretical study on OH-(H₂O)_n n=0-7?
K. Takahashi*

9:40 – 121. Performance of local correlation methods for halogen bonding: The case of Br₂(H₂O)_n, n=4,5 clusters and Br₂(H₂O)₆ clathrate cage.
R. Hernandez*

10:00 Break

10:15 – 122. Stereochemical effects in spectroscopy and photostability of biomolecules.
A. Zehnacker-Renten*

10:40 – 123. Photoelectron circular dichroism of molecular cluster anions.
T. NAGATA

11:05 – 124. Understanding spectral signatures of large amplitude vibrations and hydrogen-bonding through studies of the vibrational spectroscopy of solvated ion complexes.
A.B. McCoy, L.C. Dzugan

Tuesday Afternoon

Hawaii Convention Center
308A

Ultrafast Intense Laser Chemistry (#35)

Organized by: K. Yamanouchi, R. Levis, F. Legare, Q. Gong
Presiding: R.J. Levis

13:00 – 125. Observation of attosecond quantum wavepacket dynamics in molecules.
K. Midorikawa*

13:25 – 126. Attosecond probing of chemical dynamics.
S.R. Leone*

13:50 – 127. High harmonic spectroscopy reveals electronic structure of small molecules.
D.M. Villeneuve*

14:15 – 128. Circularly polarized MOHGs (molecular high order harmonic generation) and attosecond laser pulses - new tools in laser science.
A.D. Bandrauk*

14:40 – 129. Probing molecular chirality on sub-femtosecond time scale.
O. Smirnova*, R. Cirera, A.E. Boguslavskiy, B. Pons, M.C. Wong, D. Descamps, S. Petit, A. Ferre, N. Thiré, B.E. Schmidt, A. Alharbi, F. Légaré, V. Blanchet, B. Fabre, J. Suarez, J. Higuet, H. Ruf, A. Harvey, M. Richter, F. Morales, M. Ivanov, S. Patchkovskii, Y. Mairesse, R. Bhardwaj

15:05 Break

15:20 – 130. Laser-induced electron wave packets as a sub-nanometer and sub-femtosecond molecular probe.
L.F. DiMauro*, C.I. Blaga, J. Xu

15:45 – 131. Strong-field ionization and dissociation dynamics in heterocyclic aromatic molecules probed by femtosecond XUV transient absorption spectroscopy.
F. Lackner*, A.S. Chatterley, S.C. Pemmaraju, D. Neumark, S.R. Leone, O. Gessner

16:00 – 132. Two-photon non-sequential double ionization pathway of Ar with anomalous selectivity.
K. Yamada, A. Iwasaki, T. Sato, K. Midorikawa, K. Yamanouchi*

* Principle Author

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16:15 – 133. Multiphoton ionization of He, Ne, Ar, and Xe using full-coherent free electron laser seeded by high-order harmonics of near-infrared femtosecond laser pulses. **A. Iwasaki**, S. Owada, S. Ogami, T. Togashi, E.J. Takahashi, K. Midorikawa, M. Aoyama, K. Yamakawa, S. Matsubara, K. Ogawa, Y. Okuyasu, H. Tomizawa, T. Watanabe, M. Nagasomo, M. Yabashi, T. Ishikawa, K. Yamamoto
16:30 – 134. Single-shot photoelectron spectroscopy of nonlinear ionization of He in intense EUV FEL fields. Y. Hikosaka*, M. Fushitani, A. Matsuda, T. Endo, Y. Toida, E. Shigemasa, A. Hishikawa*
16:45 – 135. Ultrafast two-photon Rabi oscillations in excited He driven by femtosecond intense laser fields. **M. Fushitani**, C. Liu, A. Matsuda, T. Endo, Y. Toida, Y. Hikosaka, T. Morishita*, A. Hishikawa*

Hawaii Convention Center
301A

Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60)

Organized by: A. Kovalenko, B. Pettitt, F. Hirata
Presiding: A. Kovalenko, M. Pettitt

13:00 – 136. Characterization of the GroEL – GroES interface and the mechanism of reversible chaperonin association. **P.J. Rossky**, C. Bajaj, L.H. Kapcha
13:30 – 137. Multiscale modeling using molecular theory of solvation: Effective forces from statistical-mechanical ensemble of atomic interactions. A. Kovalenko*

14:00 – 138. Structural fluctuation of protein induced by thermodynamic perturbation. F. Hirata

14:30 – 139. Predicting protein motion from structural ensembles: A coarse-grained model of protein dynamics. **M. Guenza**, J.T. Copperman

15:00 – 140. Molecular theory of solvation: From heavy petroleum to plant biomass valorization. **S. Stoyanov**, A. Kovalenko

15:15 Coffee Break

15:30 – 141. DPD with an effective pair potential from integral equation theory of molecular liquids. **A.E. Kobryn**, S. Gusalov, A. Kovalenko

15:45 – 142. Evaluation of effective interactions of kaolinite nanoparticles in aqueous electrolyte solution with polymer by molecular theory of solvation. S. Hlushak, S. Stoyanov, A. Kovalenko*

16:00 – 143. Analyzing the binding free energy for the inclusion process of 2-hydroxypropyl- β -cyclodextrin by means of the MD/3D-RISM method. **M. Sugita**, F. Hirata

16:15 – 144. Solvation effects in pathological conversion of proteins implicated in neurodegeneration: Insight from the 3D molecular theory of solvation. **N. Blinov**, N. Cashman, A. Kovalenko

16:30 – 145. Water and Mg²⁺ ion distributions in EcoRV-DNA complex prior to and after endonuclease-reaction calculated by using 3D-RISM. **M. Iriya**, R. Motomatsu, S. Sunaba, J. Yasuniwa, Y. Maruyama, N. Yoshida, A. Sarai, F. Hirata

17:00 – 146. High accuracy solvation enthalpies, entropies, and free energies from 3D-RISM. **T. Luchko**, J. Johnson, T. Yamazaki, S. Gusalov, A. Kovalenko, D. Case

Hawaii Convention Center
308B

New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems (#84)

Organized by: T. Carrington, J. Bowman, D. Zhang
Presiding: S. Manzhos

13:00 – 147. Electronic structure and potential fitting methods suitable for multistate reactive surfaces. **R. Dawes***
13:30 – 148. Large scale exact quantum dynamics calculations: Massive parallelization and the classical phase space picture. **B. Poirier***
14:00 – 149. Mixed quantum/classical treatment of the ozone forming reaction. D. Babikov*

14:18 BREAK

14:38 – 150. Simple parameterization of the quantum energies, rotational constants, and centrifugal distortion constants of Lennard-Jones m - n potentials. R.B. Shirts*

14:56 – 151. Quantum and isotope effects in water clusters. **V. Mandelstham**, S.E. Brown*, J. Mallory*
15:26 – 152. Efficient treatment of coupled large amplitude motions using analytic integrals. W.A. Kopp*, M. Döntgen, K. Leonhard

15:44 – 153. New approaches to simulating biological and molecular catalysts. T.F. Miller

16:14 – 154. On the fly semiclassical dynamics. E. Pollak

16:44 – 155. Dynamical effects on multistep reactions with unstable intermediates. G. Jimenez-Oses, L. Törk, C. Doubleday, K.N. Houk

Hawaii Convention Center
305B

Deciphering Molecular Complexity from Single Molecules to Cellular Networks (#121)

Organized by: T. Komatsuzaki, J. Wang, J. Wu
Presiding: S. Pressé, S. Takada

13:00 – 156. Energy landscape theory: From folding proteins to folding chromosomes. P.G. Wolynes*

13:35 – 157. Enzymes stepping on landscapes. S. Pressé

14:05 – 158. Enhanced sampling and applications in protein folding in explicit solvent. J. Ma*

14:35 BREAK

14:50 – 159. Dynamical energy landscape perspective on protein functioning. M. Sasai*, T.P. Terada, Q. Nie

15:25 – 160. Energy landscapes and conformation network learned from single molecule time series. **T. Komatsuzaki***

15:55 – 161. Modes of protein large-amplitude conformational change from single-molecule experiments. H. Yang

16:25 – 162. Signal and information processing with biomolecules: Enzyme-catalyzed reactions and their cascades. V. Privman*

Hawaii Convention Center
305A

Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130)

Organized by: A. Wilson, P. Schwerdtfeger, K. Kim, Z. Lin, T. Cundari
Presiding: Z. Lin

13:00 – 163. Advances in GVPT multireference perturbation theory: Transition metals and lanthanides. M.R. Hoffmann*, P.K. Tamukong, W. Liu

13:30 – 164. Efficient and size-insensitive multireference description of the electronic excited states of molecules and nanomaterials. B.G. Levine, B.S. Fales, E.G. Hohenstein, Y. Shu

14:00 – 165. Developments for heavy element chemistry: Towards thermochemical prediction. A. Wilson

14:45 – 166. Tackling the challenges of modeling f-electron species in realistic environments. W.A. de Jong, N. Govind, E.J. Bylaska, R. Atta-Fynn

15:15 – 167. Designing extractants for separation of critical materials. T. Windus, V. Bryantsev, N. De Silva, M. Dick-Pérez, M.S. Gordon, B. Hay, B. McCann, F. Zahariev

15:45 – 168. Relativistic open-shell Hartree-Fock theory with time-reversal symmetry. M. Nakano*, R. Nakamura, J. Seino, H. Nakai

16:05 – 169. Theoretical studies of rare earth CeO₂ catalysis. X. Gong, X. Wu, L. Yin, G. Lu, J. Zhang

16:25 – 170. Bonding and structure of redox non-innocent ligands, and their use to “ennoble” base metal catalysts. T. Cundari

Hawaii Convention Center
306B

Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134)

Organized by: P. Piotrowiak, M. Fujii, J. Tang, B. Zhang
Presiding: M. Sakai, J. van de Lagemaat

13:00 Opening remarks

13:05 – 171. Feeling fast charge carriers: Time-resolved electrostatic force microscopy for solar cells. D. Ginger*

13:45 – 172. Probing the effect of a surface plasmon on the exciton dynamics in a single quantum dot by simultaneously trapping a metal nanoparticle with a quantum dot in a topological singularity. P.J. Ackerman, H. Mundoor, I.I. Smalyukh, J. van de Lagemaat*

14:25 – 173. Sub-femtosecond time-resolved photoemission electron microscopy of propagating surface plasmons. W. Hess, Y. Gong*, A. Joly, d. Hu, P. El-Khoury

15:05 BREAK

15:20 – 174. Nanoscopic visualization of stacking domains of few-layer graphene infrared near-field microscopy. Z. Kim*

16:00 – 175. Multistage plasmonic nanofocusing NSOM-Raman tip for high resolution chemical mapping. R. Yan*

16:30 – 176. Influence of polarized light on metal nanoparticle-originating high resolution TIRF imaging. A. Ishijima*, P. Wang, S. Ryuzaki, K. Okamoto, K. TAMADA

Hawaii Convention Center
313C

Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)

Organized by: J. Hasegawa, M. Collins, M. Gordon, P. Piecuch, T. Taketsugu
Presiding: J. Hasegawa

13:00 – 177. Multireference methods for excited-states of molecular systems. L. Gagliardi*, R. Carlson, K. Vogiatzis, D.G. Truhlar

13:30 – 178. Relativistic multiconfiguration methods for excited states. H. Nakano*

14:00 – 179. Relativistic equation-of-motion coupled-cluster theory. F. Wang

14:20 – 180. Two-component relativistic effects for excited states: Energies and oscillator strengths. F. Egidi*, J. Goings, X. Li

14:40 – 181. Exploration of excited state potential surfaces of photofunctional molecules using the Global Reaction Route Mapping (GRRM) strategy. K. Morokuma*

15:10 – 182. Modelling the photoisomerisation and photodissociation of acetaldehyde. M.J. Jordan*, M. Corrigan, S. Kable

15:40 – 183. Excited states of the Si/C-alternately mixed annulenes. T. Kudo

16:10 – 184. Theoretical insight into the photodissociation mechanism of methyl formate. H. Xiao

16:30 – 185. Automated search for minimum energy conical intersection and seam of crossing geometries near the Franck-Condon region: Toward prediction of fluorescence quantum yields. Y. Harabuchi*, T. Taketsugu, S. Maeda

Hawaii Convention Center
313A

Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168)

Organized by: A. Terasaki, S. Anderson, N. Gaston
Presiding: M. Ichihashi

13:00 – 186. Ligand-protected gold superatoms and superatomic molecules. T. Tsukuda*

13:30 – 187. Investigating the role of phosphines in the synthesis and stability of gold clusters. G.E. Johnson*

13:50 – 188. Ligand-mediated control of the surface plasmon resonance in metal nanoparticles generated by laser ablation. A. Mulder, R. Tilbury, M. Werrett, P. Wright, M. Massi, P. Raiteri, M. Buntine

14:10 – 189. Unique optical properties of shape-controlled gold clusters: Surprising correlation between geometric and electronic structures. Y. Shichibu*, M. Zhang, K. Konishi

14:30 – 190. The quest for highly efficient photocathodes. I.J. Macdonald, S. Chandrasekaran, A. Fonseka, H. Tan, C. Jagadish, N.H. Voelcker, T. Nann*

15:00 break

15:15 – 191. Adsorption and desorption of hydrogen by gas-phase palladium clusters revealed by in-situ thermal desorption spectroscopy. M. Takenouchi, S. Kudo, K. Miyajima, F. Mafune*

15:45 – 192. Effect of metal-organic framework on the kinetics of hydrogen absorption in Pd@HKUST-1. T. Tsutsumi, T. Ishimoto, M. Koyama

16:05 – 193. Structure, stability, and electronic properties of neutral and charged zinc clusters containing up to 73 atoms. A. Aguado*, A. Vega, A. Lebon, B. von Issendorff

16:25 – 194. Percolating films of clusters. S. Brown

Hawaii Convention Center
304A

Theory of Main Group Chemistry Beyond First Row (#183)

Organized by: T. Dunning, M. Gordon, P. Schwerdtfeger, C. Choi
Presiding: M.S. Gordon

13:00 – 195. Gallium, a molecular metal: Nanoscale and finite temperature effects on bonding. N. Gaston*, K.G. Steenbergen

13:30 – 196. Electronic structures and spectroscopy of adsorbates on semiconductor surfaces: From small clusters to infinite lattices. K. Raghavachari

14:00 – 197. Synergy between experiment and theory: Low valent main group cations and tetrelenes. K.M. Baines*

* Principle Author

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14:30 – 198. Mesoporous silica nanoparticles: Transcending single molecule confinement to understand cluster confinement. **I.I. Slowing**

15:00 – 199. Donor-acceptor adducts of aminocarbenes with silylenes: Predicting the synthesis of novel silenes ($R_2Si-CR'_2$). **Y. Apeloig**

15:30 – 200. Gold surfaces and nanoparticles are protected by Au(I)-thiol species but not Au(I)-thiolates. **J. Reimers***, J. Ulstrup, N.S. Hush

16:00 – 201. Simulation of phase transitions with highly accurate ab initio potentials: Applications to argon. **E. Pahl***, J. Wiebke, P. Schwerdtfeger

Hawaii Convention Center
304B

Latest Development of Advanced Vibrational Spectroscopy (#187)

Organized by: K. Iwata, S. Asher, D. Phillips, Y. Furukawa
Presiding: L.A. Nafie, D.L. Phillips

13:00 – 202. Electronic and spectroscopic properties of avobenzone derivatives attached to Mg quadruple bonds: Implications for the photochemical enol to keto transformation. M.H. Chisholm, C.B. Durr, **T.L. Gustafson***, W.T. Kender, T.F. Spiller, P.J. Young

13:25 – 203. Tuning excited state properties of dpzp complexes with donor substituents: A computational and spectroscopic study. **K.C. Gordon***

13:50 – 204. Time-resolved vibrational spectroscopic studies of the photochemistry of selected drugs and phototrigger compounds. **D.L. Phillips***

14:15 – 205. Time-resolved infrared studies of cyclopentane-1,3-diyli diradicals. **T. Ishibashi***

14:40 – 206. Time-resolved frequency analysis of excited state ab initio dynamics to understand THz-IR signals in photoreactivity and relaxation processes. **N. Rega***

14:55 break

15:05 – 207. Low-frequency vibrational modes and intermolecular interaction of Nylon 6 studied by Raman, far-IR, and terahertz spectroscopies with quantum chemical calculation. **Y. Ozaki***, E. Onishi, S. Yamamoto, H. Sato, D. Ishikawa, H. Hoshina

15:30 – 208. Low-frequency vibrations of molecular crystals investigated by terahertz spectroscopy and solid-state density functional theory calculation. F. Zhang, M. Hayashi, **K. Tominaga**

15:55 – 209. Probing intermolecular interactions of core fragments of β_2 -microglobulin amyloid fibrils with low-frequency Raman spectroscopy. **S. Shigeto***, C. Chang, H. Chen, H. Hirayama

16:15 – 210. Vibrational quantum beats in pure liquids measured with ultrafast terahertz Kerr effect spectroscopy. **M.A. Allodi***, I.A. Finneran, G. Blake

16:30 – 211. Hydrogen bonding in mixtures of ionic liquids. **S. Cha***, D. Kim

16:45 – 212. Probing the structure of protonated water solvates in acetonitrile by FTIR and 1H NMR. **E. Pines***

Hawaii Convention Center
301B

Frontier Chemical Applications Using Accelerator Based Photon Sources (#414)

Organized by: K. Asakura, T. Sham, L. Chen
Presiding: T.K. Sham

13:00 – 213. Hydrogen-related properties of metal and alloy nanoparticles. **M. Yamauchi***

13:20 – 214. Visualizing electronic and structural dynamics in transition metal complexes by XFEL sources. **M.M. Nielsen***

13:50 – 215. Ultrafast X-ray transient spectroscopy using LCLS. M.L. Shelby, M.W. Mara, N.E. Jackson, A.B. Stickrath, **L.X. Chen***, P.J. Lestrage, X. Li

14:10 – 216. Dynamics of the photoexcited WO_3 in the time scale from femtoseconds to nanoseconds. **Y. Uemura**, D. Kido, Y. Wakisaka, H. Uehara, T. Ohba, Y. Niwa, S. Nozawa, T. Sato, K. Ichianagi, R. Hukaya, S. Adachi, T. Katayama, T. Togashi, K. Ogawa, M. Yabashi, S. Takakusagi, T. Yokoyama, B. Ohtani, K. Asakura

14:25 Break

14:40 – 217. Site specific solvation dynamics of a model photocatalyst studied with ultrafast diffuse X-ray scattering. **K. Gaffney***, M.M. Nielsen, K. Moller, a. dohn, K. Haldrup, T. Harlang, R. Hartsack, K. kjaer, H. Lemke, T. van Driel, W. Zhang

15:10 – 218. Ultrafast molecular structural dynamics of metal complexes probed by time-resolved X-ray experiments. **S. Nozawa**

15:40 – 219. Freezing reactive ions in time: Nonlinear optical imaging of the spatial distribution of X-ray induced ions. **G. Simpson***

16:00 – 220. Liquid flatjet system for solution phase soft-X-ray spectroscopy. M. Ekinova, W. Quevedo, M. Faubel, P. Werner, **E. Nibbering***

16:20 – 221. Studying band gap engineering in materials using resonant X-ray emission spectroscopy. **J. McLeod***, A. Moewes, E. Kurmaev

Hawaii Convention Center
306A

Frontiers of Photon Upconversion Based on Triplet-triplet Annihilation (#420)

Organized by: P. Zhang, Y. Murakami, J. Zhao
Presiding: Y. Murakami, P. Zhang, J. Zhao

13:00 – 222. Toward efficient photon upconversion: Plasmonic and covalent tethering strategies. **T. Kelly***

13:30 – 223. Triplet energy migration in self-assembled molecular systems for efficient photon upconversion. **N. Yanai***, N. Kimizuka

13:50 – 224. Design of organic triplet photosensitizers and applications in triplet-triplet annihilation upconversion. **J. Zhao**

14:10 – 225. Analytical and statistical analysis of power-dependent NIR to visible upconversion from $NaYF_4: Yb^{3+}, Er^{3+}$ nanoparticles on Au nano-cavity arrays. **S. Smith***

14:40 Break

14:55 – 226. Assessing photodamage in triplet-triplet annihilation-based upconverting polymer films. **M. Paige**, C. Ponce, A.M. Pereira, N. Joshi

15:15 – 227. Large distance interaction during triplet-triplet annihilation process. A. Sakurai, Y. Sakagami, Y. Fujiwara, K. Kobayashi, **K. Kamada***

15:35 – 228. New chromophore systems for near infrared-to-visible and visible-to-UV photon upconversion. **S. Amemori***, N. Yanai, P. Duan, N. Kimizuka

15:55 – 229. Triplet-triplet annihilation upconversion using polymeric emitters. X. Yu, X. Cao, X. Chen, N. Ayres*, **P. Zhang***

16:15 Concluding remark

Hawaii Convention Center
313B

Computational Modeling of Magnetic Materials and Magnetic Properties (#423)

Organized by: J. Peralta, A. Soncini, T. Nakajima
Presiding: T. Nakajima, J. Peralta

13:00 – 230. Time-dependent two-component density functional theory. **X. Li**

13:30 – 231. Correlating magnetic exchange in dinuclear bis-(phenolate) bridged complexes: A computational perspective. **A. Velloth**, H. Sakiyama, M. Hada

13:40 – 232. Landing functional molecular spin clusters on surfaces. **M. Affronte***

14:10 – 233. Spin-orbit-assisted correlations and novel magnetic ground states and excitations in 5d oxides. L. Hozoi*, **R. Yadav**

14:20 – 234. Magnetism and electronic structure at perovskite fluoride-based interfaces. **a.h. romero***, A.C. Garcia-Castro, E. Bousquet

14:50 Coffee Break

15:10 – 235. Molecular spin filters and polarizers. **V. Mujica***

15:40 – 236. Calculation of isotropic exchange coupling constants with density functional theory. **A. Mansikkamäki***, H.M. Tuononen

15:50 – 237. Spin torque and zeta force in molecules and magnetic materials. **M. Senami***, M. Fukuda, K. Soga, A. Tachibana

16:00 – 238. From structures and magnetic tensors to full EPR spectra of large free radicals in different environments. **V. Barone***

Hawaii Convention Center
310 Theatre

Frontiers of Plasmon Enhanced Spectroscopy (#428)

Organized by: Y. Ozaki, Z. Tian, B. Ren, N. Halas, A. Brolo, T. Itoh, M. Moskovits
Presiding: D. Graham, T. Itoh

13:00 – 239. Nanoparticle based analysis of biomolecules, cells, and tissue. **D. Graham***, K. Faulds, S. Mabbott, J. Simpson, H. Kearns

13:20 – 240. Shell-isolated nanoparticle-enhanced spectroscopy. **J. Li***, S. Ding, Z. Yang, C. Li, **Z. Tian**

13:40 – 241. Electrochemical reactions on plasmonic nanoparticle electrodes. **K. Willets**

14:00 – 242. Driving and following surface chemical reactions of individual molecules with gap-plasmons. **Z. Kim***

14:20 – 243. Molecule trapping monitored by surface-enhanced Raman scattering spectroelectrochemistry. **K. Murakoshi***

14:40 – 244. Structural and optical properties of linear chains of plasmonic nanocubes. **E. Kumacheva**

15:00 Break

15:15 – 245. Extreme enhancement factors: Application of surface enhanced spectroscopy to nonlinear light scattering. **J. Camden***

15:35 – 246. What can we learn from single molecule SERS? **A.G. Brolo**, D. dos Santos, M. Temperini

15:55 – 247. Electromagnetic strong coupling system composed of Ag nanoparticle dimer and dye molecules evaluated by a classical coupled-oscillator model. **T. Itoh***, Y.S. Yamamoto, H. Tamari, V. Biju, S. Wakida, Y. Ozaki

16:15 – 248. Single-molecule SERS: A multi-analyte comparison of the bimanalyte and isotopologue proofs. **A.B. Zrimsek**, N.L. Wong, R.P. Van Duyne*

16:30 – 249. Chemical enhanced effect of surface-enhanced Raman spectroscopy of aromatic compounds in electrochemical interfaces. **T. Wu**, X. Jin, **D. Wu**, Z. Tian

16:45 – 250. Tunneling-plasmon-induced Raman spectroscopy. **K. Rodriguez**, M. Banik, E. Hulkko, S. Dey, V.A. Apkarian*

Hawaii Convention Center
307AB

Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)

Organized by: H. Sekiya, T. Zwier, M. Fujii, E. Bieske, N. Kim
Presiding: M. Fujii, T.S. Zwier

13:00 – 251. Correlating photoacidity to hydrogen-bond structure by use of the local O-H stretching probe in hydrogen-bonded complexes of aromatic alcohols. B.T. Psciu, M. Prémont-Schwarz, B. Koeppe, S. Keinan, D. Xiao, V. Batista, **E. Nibbering***

13:25 – 252. Computational investigation of the vibrational spectra of ionic aqueous clusters: The OH stretch as a signature of water patterning by sulfate ions. X. Wang, **G.H. Peslherbe**

13:45 – 253. Structure and dynamics of charge accommodation by H-bonded water networks with temperature-dependent IR -IR double resonance. **M.A. Johnson**

14:10 – 254. Spectroscopic investigation on the hydration structure of the temperature-controlled molecular cations. **H. Ishikawa***, R. Yagi, I. Kurasu, Y. Kasahara

14:30 – 255. Role of the hydrogen bonds in the excited state dynamics of protonated molecules. **G. Féraud, C. Dedonder**, M. Broquier, G. Gregoire, S. Soorkia, C. Jouvet

14:55 Break

15:10 – 256. Spectroscopic studies of jet-cooled acetaminophen-water clusters. **M. Choi***, A. Min, A. Ahn, C. Moon, J. Lee

15:30 – 257. Excited state dynamics of nucleobase clusters. **M.S. de Vries***

15:55 – 258. Gas phase spectroscopy of neurotransmission system by laser desorption supersonic jet technique. **S. Ishiuchi**, M. Fujii

16:15 – 259. Probing the dipole-bound excited state of cold anions by temperature controlled electrospray ionization combined with photoelectron imaging. **H. Liu**, L. Wang

Wednesday Morning

Hawaii Convention Center
308A

Ultrafast Intense Laser Chemistry (#35)

Organized by: K. Yamanouchi, R. Levis, F. Legare, Q. Gong
Presiding: F. Légaré

8:00 – 260. Ultrafast imaging of molecular deformation induced by intense laser fields. **K. Yamanouchi***

8:25 – 261. Periodical H_3^+ emission from CH_3OH^{2-} by pump-probe coincidence momentum imaging using few-cycle intense laser pulses. **T. Ando**, A. Shimamoto, S. Miura, A. Iwasaki, K. Yamanouchi*

8:40 – 262. Strong-field double ionization of acetylene. **J. Wu**

9:05 – 263. Strong field molecular ionization with shaped laser pulses. **T. Weinacht***

9:30 – 264. Mass-resolved ion beam apparatus for investigating dissociation dynamics of molecular ions in intense laser fields. **T. Yamazaki**, K. Fujiwara, R. Kanya, K. Yamanouchi*

9:40 – 265. Pulse duration dependence of Coulomb explosion of formaldehyde in intense laser fields studied by triple ion coincidence momentum imaging. **M. Fushitani**, C. Tseng, A. Matsuda, A. Hishikawa*

9:55 Break

* Principle Author

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10:10 – 266. Directionally asymmetric molecular tunneling ionization by four-color Fourier-synthesized laser fields.
H. Ohmura*, N. Saito

10:25 – 267. Intensity and wavelength dependence of intense field ionization of aligned N_2 molecules.
H. Hasegawa*, S. Kimura, T. Sato, A. Iwasaki, K. Yamanouchi

10:40 – 268. Direct and detailed characterization of unidirectional molecular rotation using a newly developed ion imaging apparatus.
K. Mizuse*, Y. Ohshima

10:55 – 269. First-principles simulation of the reaction dynamics and Coulomb explosions of C_{60} induced by ultrashort intense laser pulses.
H. Kono*, K. Yamazaki, Y. Takehara, N. Nitsu, W.C. Chung, M. Kanno, K. Ueda

11:20 – 270. Dynamics of H_2He^+ in intense laser fields.
T.J. Szidarovsky*, K. Yamanouchi

11:35 – 271. Obtaining insights into the dynamics of radical cations produced via strong field ionization.
S. Matsika*, M. Assmann, T. Weinacht, H. Koeppl

Hawaii Convention Center
301A

Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60)

Organized by: A. Kovalenko, B. Pettitt, F. Hirata
Presiding: F. Hirata, A. Kovalenko

8:00 – 272. Multiscale couplings for chemical processes at molecular level: Quantum chemistry and statistical mechanics.
H. Sato*

8:30 – 273. Molecular modeling of ionic liquids.
A. Yethiraj*

9:00 – 274. Liquid state theory for dynamics of electrochemical materials.
T. Yamaguchi*

9:30 – 275. Density-based adaptive QM/MM method for modeling explicitly solvated systems.
M.P. Waller

9:45 – 276. Predictive calculations of redox potentials of solvated molecules: A combined QM/EPP/PCM approach.
K. Bravaya, R. Tazhigulov

10:00 Coffee Break

10:15 – 277. Optimization of combination of 3D reference interaction site model with density functional theory.
G. Sergei*

10:30 – 278. Multiscale implementation of 3D-RISM to the electronic structure theory being applicable for solvated biomolecules.
N. Yoshida*

11:00 – 279. Modeling bridging water in binding association: Where do we stand?.
J. Truchon*, S. Chahal

11:30 – 280. Molecular density functional theory for water with liquid-gas coexistence and correct pressure.
G. Jeanmairet, M. Levesque, V. Sergievskiy, **D. Borgis**

Hawaii Convention Center
308B

New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems (#84)

Organized by: T. Carrington, J. Bowman, D. Zhang
Presiding: R. Dawes

8:00 – 281. Molecular dynamics of large systems with quantum corrections for the nuclei.
S. Garashchuk*

8:30 – 282. Vibrational SCF and correlation theories with optimized coordinates.
K. Yagi*

9:00 – 283. Multilayer sum-of-products method for computing vibrational spectra without storing full-dimensional vectors or matrices.
T. Carrington, P. Thomas

9:30 Break

9:50 – 284. Theoretical model of the vibrational spectroscopy of benzene-(water) n clusters with $n = 3-7$.
D.P. Tabor, **E.L. Sibert***, P.S. Walsh, R. Kusaka, T.S. Zwier

10:20 – 285. Self-consistent phonons with quasi-Monte Carlo: An efficient approach for computing thermodynamic and dynamic properties of high-dimensional systems.
S.E. Brown*, V. Mandelshtam

10:40 – 286. Hamiltonian algorithm and its application on the optimization of the structures of monoethanolamine and its water complexes.
H. Teramae*, Y.Y. Maruo

11:00 – 287. Chemical dynamics on high-dimensional ab initio potential energy surfaces.
J. Bowman*, Y. Wang, X. Wang, R. Conte, C. Qu

Hawaii Convention Center
305B

Deciphering Molecular Complexity from Single Molecules to Cellular Networks (#121)

Organized by: T. Komatsuzaki, J. Wang, J. Wu
Presiding: J. Cao, H. Yang

8:00 – 288. Dynamics and mechanism of UV-perception by UVR8 photoreceptor.
D. Zhong*

8:30 – 289. Data-driven quantification of heterogeneous microenvironments in live-cell Raman microscopic images.
J.N. Taylor, C. Li, A. Palonpon, K. Fujita, T. Komatsuzaki

8:45 Break

9:00 – 290. Structural insights into chromatin folding and transcriptional regulation.
S. Takada*

9:35 – 291. Human genome organization and dynamics: Local nucleosome dynamics facilitate chromatin accessibility.
K. Maeshima*

10:05 – 292. Beyond Förster resonant energy transfer theory.
J. Wu

Hawaii Convention Center
305A

Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130)

Organized by: A. Wilson, P. Schwerdtfeger, K. Kim, Z. Lin, T. Cundari
Presiding: T.R. Cundari

8:00 – 293. On the highest oxidation state in actinide compounds.
J. Li*

8:30 – 294. Accurate first principles calculations of the surface electronic structure of GdN .
N. Gaston*

9:00 – 295. Novel aspects of lanthanide and actinide chemistry.
P.S. Bagus, C.J. Nelin

9:30 BREAK

9:45 – 296. Theoretical study of the thermo-sensitive f-1 emission and quenching in lanthanide compounds.
M. Hatano*

10:15 – 297. Structure and vibrations of lanthanide trifluoride (LnF_3) embedded in noble gas matrix: Application of large-scale ab initio relativistic molecular orbital theory.
H. Mori, A. Matsuda, M. Klobukowski

10:45 – 298. Lanthanide and actinide ions with valenced electron configuration.
F. Furche*, G.P. Chen, A.K. Chan

11:15 – 299. Relativistic theory of active components in organic light-emitting diodes.
J. Gonzalez, A.R. Smith, P.L. Burn, B. Powell*

Hawaii Convention Center
306B

Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134)

Organized by: P. Piotrowiak, M. Fujii, J. Tang, B. Zhang
Presiding: L. Gundlach, S. Koshihara

8:00 Session opening remarks

8:05 – 300. Ultrafast multidimensional photoelectron imaging of real and reciprocal space electron dynamics at metal surfaces.
H. Petek*

8:45 – 301. Role of the femtosecond time-resolved photoemission electron microscopy for the imaging of photogenerated carrier dynamics.
S. Koshihara*, K. Fukumoto, K. Onda

9:15 – 302. Observation of plasmonic wavepacket dynamics by ultrafast time-resolved near-field imaging.
Y. Nishiyama*, K. Imura, H. Okamoto

9:45 Break

10:00 – 303. Ultrafast probe of charge carrier dynamics and lasing in single II-VI nanowires.
L. Gundlach, P.S. Eldridge, J. Blake

10:30 – 304. Using ultrafast optical microscopy to unravel carrier dynamics in semiconductor nanowires.
R.P. Prasankumar*

11:00 – 305. Polarization- and phase-sensitive vibrationally resonant sum frequency generation microscopy.
Y. Han, J. Hsu, V. Raghunathan, E. Potma, **N. Ge***

11:30 – 306. Ethanol vapor imaging system "sniffer camera" with UV-LED excitation sheet for monitoring of alcohol metabolism from human.
P. Chien, Y. Mei, K. Itani, T. Sato, K. Toma, T. Arakawa, K. Mitsubayashi*

Hawaii Convention Center
313C

Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)

Organized by: J. Hasegawa, M. Collins, M. Gordon, P. Piecuch, T. Taketsugu
Presiding: T. Taketsugu

8:00 – 307. Coupled electronic and nuclear dynamics in excited states.
K. Takatsuka*

8:30 – 308. New Gaussian basis set methods for multistate dynamics.
T.J. Frankcombe*

9:00 – 309. Exploration of chemical reactions driven by non-adiabatic electron wave packets created in densely quasi-degenerate electronic states.
T. Yonehara*

9:20 – 310. Internal conversion of molecular crystals.
M. Hayashi*

9:50 – 311. Conical intersections and nonradiative recombination in semiconductor nanocrystals.
B.G. Levine, B.S. Fales, G.A. Meek, Y. Shu

10:20 – 312. Charge carrier generation and transport in oxide perovskites from first-principles localized chemical models.
M. Dupuis*, N. Tyminska, G. Wu

10:50 – 313. Representation of adiabatic potential energy surfaces coupled by conical intersections: Construction and use.
X. Zhu, C.L. Malbon, **D.R. Yarkony***

11:20 – 314. Novel approaches to nonadiabatic molecular dynamics.
O. Prezhdo

Hawaii Convention Center
313A

Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168)

Organized by: A. Terasaki, S. Anderson, N. Gaston
Presiding: N. Gaston

8:00 – 315. Size-selected gold clusters: Solving the atomic structure of model nanoparticles then scaling-up production.
R.E. Palmer*

8:30 – 316. Genetically encoded nanocluster assemblies: Photophysics and catalytic function.
J.S. Martinez*, A. Desiraju, S. Chakraborty, S. Babanova, A.P. Shreve, E. Balog, R.C. Rocha, K. Artyushkova, P. Atanassov

9:00 – 317. Steady state and time-resolved fluorescence studies on the silver nanoclusters synthesized in human telomeric DNA.
C. Chang*

9:20 – 318. Bond stiffening in icosahedral-based Au clusters.
S. Yamazoe, S. Takano, W. Kurashige, Y. Negishi, T. Tsukada*

9:40 break

9:55 – 319. Cluster magnetism with X-rays and ion traps: From high spin states of transition metal diatomics to spin and orbital magnetic moments of transition metal clusters and complexes.
T. Lau*

10:25 – 320. Melting of mercury clusters and the bulk.
E. Pahl*, P. Schwerdtfeger, F. Calvo, M. Wormit

10:55 – 321. Vibrational and low-temperature thermal properties of metal clusters and nanoparticles.
I.L. Garzon*

11:15 – 322. Intrinsic finite-size constraint on the cluster liquid state elevates melting temperatures.
K.G. Steenbergen*, N. Gaston

Hawaii Convention Center
Halls I, II, III

Theory of Main Group Chemistry Beyond First Row (#183)

Organized by: T. Dunning, M. Gordon, P. Schwerdtfeger, C. Choi
Presiding: P. Schwerdtfeger

Poster Session

10:00 – 12:00

323. Diagonal correction of Born-Oppenheimer approximation for heavy-element main-group molecules with scalar-relativistic Hamiltonians.
M. Abe*, Y. Imafuku, M.W. Schmidt, M. Hada

324. ^{13}C - and ^{207}Pb -NMR chemical shifts of dihydro and dilithioplumbole complexes: A quantum-chemical assessment.
R. Narayanan Nair, M. Nakada, M. Saito, M. Hada

325. Computational study of the gas-phase reactivity of 2-iodoethanol with homo- and hetero-metallic hydride clusters of silver and copper.
S.S. Leang*, M.S. Gordon, G. Khairallah, R. O'Hair

326. Theoretical study on the ligand exchange and ligand coupling reactions of hypervalent Sb and Te compounds.
M. Kobayashi*, Y. Kuroda, K. Akiba, T. Taketsugu

327. Geometries and molecular properties of heavy-element molecules based on efficient and accurate two-component relativistic scheme.
Y. Nakajima*, J. Seino, H. Nakai

Hawaii Convention Center
304B

Latest Development of Advanced Vibrational Spectroscopy (#187)

Organized by: K. Iwata, S. Asher, D. Phillips, Y. Furukawa
Presiding: P. Champion, T. Ishibashi

8:00 – 328. Ultrafast measures of energy relaxation and solvation in lipids, water, and supercritical fluids.
L. Ziegler*

8:25 – 329. Temporal Raman mapping of vibrational energy flow in hemoprotein.
Y. Mizutani*

8:50 – 330. Relaxation of the OH stretching overtones in isolated HDO molecules observed by IR pump-repump-probe spectroscopy.
D. Hutzler*, J. Werhahn, R. Heider, m. bradler, R. Kienberger, E. Riedle, H. Iglov

9:05 – 331. Characterizing lipid bilayer membranes with time-resolved spectroscopies.
Y. Nojima, S. Kitamura, T. Takaya, **K. Iwata***

* Principle Author

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- 9:30 – 332.** Mixed quantum/classical approach for predicting amide vibrational bands of sphingomyelin bilayer. **K. Yagi***
9:55 break
10:05 – 333. An origin of complicated infrared spectra of perfluoroalkyl compounds involving a normal alkyl group. **T. Hasegawa***, T. Shimoaka, Y. Tanaka, N. Shioya, K. Morita, M. Sonoyama, H. Amii, T. Takagi, T. Kanamori
10:30 – 334. Determination of molecular interactions between silica, bitumen, and water using sum frequency generation spectroscopy. **A.M. Darlington**, J. Gibbs-Davis
10:50 – 335. Operando attenuated total reflection-infrared spectroscopic detection of the catalytic solid-liquid-gas interface during semi-batch hydrogenation. **F. Meemken***, L. Rodriguez Garcia, K. Hungerbühler, A. Baiker
11:10 – 336. Sub-wavelength resolution broadband sum frequency generation vibrational spectroscopy and coherent vibrational dynamics at molecular interfaces. **H. Wang***, L. Velarde, L. Fu
11:30 – 337. Fast structural dynamics of self-assembled monolayers on SiO₂ and gold surfaces measured with 2D IR spectroscopy. **C. Yan**, R. Yuan, J. Nishida, M.D. Fayer*
11:45 – 338. Probing molecular structures of peptides and proteins at interfaces using nonlinear and linear vibrational spectroscopic techniques. **Z. Chen***

Hawaii Convention Center
313B

Single-molecule Fluorescence Imaging (#208)

Organized by: P. Chen, T. Majima, G. Cosa
Presiding: G. Cosa, Y. Tan

- 8:00** Frontiers of methodology I
8:00 – 339. Story of single molecules, from early spectroscopy in solids, to super-resolution nanoscopy in cells and beyond. **W. Moerner***
8:25 – 340. Mapping biomolecular assemblies by super-resolution fluorescence imaging: Challenges and opportunities with dSTORM. **C.M. Yip***
8:50 – 341. Development of a new fluorescence imaging technique using diamond nanoparticles. **Y. Harada***
9:15 Break
9:30 Function and dynamics of proteins, enzymes, and DNAs
9:30 – 342. Single molecule microscopy reveals the mechanisms of noncoding RNA and DNA nanomachines. **N.G. Walter***
9:55 – 343. Building and visualising at the single molecule level DNA-based nanostructures. **G. Cosa***
10:20 – 344. Probing processes on the order of milliseconds using smFCs. **X. Zhao***
10:45 – 345. Studying ion channel structure and function using fluorescence spectroscopy. **R. Blunck***
11:10 – 346. Probing molecular mechanisms of signaling proteins with single-molecule techniques. **Y. Tan***
11:35 – 347. First observation of flickering fusion events by in vitro single-vesicle content mixing assay. **B. Gong**, B. Choi, J. Kim, D. Shetty, Y. Ko, N. selvapalam, N. Lee*, K. Kim*

Hawaii Convention Center
312

Interplay between Theory and Experiment in Catalytic Research (#277)

Organized by: M. Ehara, C. Cramer, S. Dai, C. Jones, T. Ziegler, T. Tsukuda

- 8:00** Opening
8:05 – 348. Role of computational models in the design cycle of catalysts. **C. Cramer**
8:25 – 349. Factors affecting selectivity in olefin polymerization. **P.H. Budzelaar***, G. Talarico

- 8:50 – 350.** Computer-aided design of radical polymerization catalysts and stereo-control agents. B. Noble, L. Smith, **M.L. Coote***
9:15 – 351. Ion-paired chiral ligands for asymmetric transition-metal catalysis. **T. Ooi***
9:30 – 352. Combined experimental and computational analysis reveals multiple rate-enhancing roles of water in olefin epoxidation catalyzed by methyltrioxorhenium. **S.L. Scott***, B. Goldsmith, T. Hawng, S. Seritan, B. Peters*
9:45 Break
10:00 – 353. Understanding the interplay between non-covalent interactions and anion reduction in a non-heme system. **A. Fout**, Y. Park, E. Matson
10:25 – 354. Single-site catalysis with supported tetratinium molecular clusters. **A. Katz**, D. Ertler, A. Palermo, A. Okrurt, A. Solovyov, D.A. Dixon, B. Gates
10:50 – 355. Theoretical understanding of catalysis by transition metal complex with unusual valence. **S. Sakaki**
11:15 – 356. Computational study of asymmetric C-C bond formation catalyzed by Lewis acid in aqueous media. **M. Hatanova**
11:30 – 357. Activating and deactivating catalysts using reaction discovery simulation. **P.M. Zimmerman**
11:45 – 358. Cooperative studies with experimentalists to understand/improve catalytic processes. **Z. Wang***

Hawaii Convention Center
301B

Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370)

Organized by: W. Zhao, W. Zhuang, M. Cho, G. Sholes
Presiding: W. Zhao

- 8:00 – 359.** Coherent multidimensional analogs of IR and vis/UV absorption, emission, Raman, and multiphoton spectroscopies and their applications to molecular and materials spectroscopy. **J.C. Wright***
8:25 – 360. Investigating the influence of composition on exciton dynamics in organic thin films. **D. Blank***, B. Caplins, P. Goff
8:50 – 361. Simulating, modeling, and analyzing 2D THz-Raman spectroscopies. **Y. Tanimura***
9:15 – 362. Ultrafast dynamics of excitation energy transfer and coherent oscillations in chlorosomes elucidated by 2D electronic spectroscopy. S. Jun, C. Yang, T. Kim, H. Tamiaki, H. Ihee, **J. Kim***
9:40 – 363. Structure of alanine pentapeptide investigated by 2D infrared spectroscopy and molecular dynamics simulation. Y. Feng, J. Huang, S. Kim, J. Shim, A. MacKrell, N. Ge*
10:05 Break
10:20 – 364. Elucidating multicolor processes with linear and multidimensional spectroscopy. **J.T. Fourkas**
10:45 – 365. Enzyme dynamics and their role in enzyme-catalyzed reactions. P. Pagano, Q. Guo, A. Kohen, **C. Cheatum**
11:10 – 366. Coherence in photosynthetic reaction centers. **J. Ogilvie**
11:35 – 367. Pathway selective multidimensional spectroscopy to resolve coherent dynamics in complex systems. **J. Davis***, J.O. Tollerud, A. Roobzebeh, F. Novelli

Hawaii Convention Center
Halls I, II, III

Frontier Chemical Applications Using Accelerator Based Photon Sources (#414)

Organized by: K. Asakura, T. Sham, L. Chen
Presiding: K. Asakura

- 8:00** Opening
8:05 – 384. Role of computational models in the design cycle of catalysts. **C. Cramer**
8:25 – 349. Factors affecting selectivity in olefin polymerization. **P.H. Budzelaar***, G. Talarico
- 8:50 – 350.** Computer-aided design of radical polymerization catalysts and stereo-control agents. B. Noble, L. Smith, **M.L. Coote***
9:15 – 351. Ion-paired chiral ligands for asymmetric transition-metal catalysis. **T. Ooi***
9:30 – 352. Combined experimental and computational analysis reveals multiple rate-enhancing roles of water in olefin epoxidation catalyzed by methyltrioxorhenium. **S.L. Scott***, B. Goldsmith, T. Hawng, S. Seritan, B. Peters*
9:45 Break
10:00 – 353. Understanding the interplay between non-covalent interactions and anion reduction in a non-heme system. **A. Fout**, Y. Park, E. Matson
10:25 – 354. Single-site catalysis with supported tetratinium molecular clusters. **A. Katz**, D. Ertler, A. Palermo, A. Okrurt, A. Solovyov, D.A. Dixon, B. Gates
10:50 – 355. Theoretical understanding of catalysis by transition metal complex with unusual valence. **S. Sakaki**
11:15 – 356. Computational study of asymmetric C-C bond formation catalyzed by Lewis acid in aqueous media. **M. Hatanova**
11:30 – 357. Activating and deactivating catalysts using reaction discovery simulation. **P.M. Zimmerman**
11:45 – 358. Cooperative studies with experimentalists to understand/improve catalytic processes. **Z. Wang***

Poster Session

10:00 – 12:00

- 368.** Time-resolved spatial distribution analysis of electrode reaction by means of vertically dispersive XAFS technique. **M. Katayama**, R. Miyahara, H. Yamagishi, S. Yamashita, Y. Inada*
369. Study on the structural change of WO₃ in its photoexcited state using picosecond W L_{2,3}-edge XANES. **D. Kido**, Y. Uemura, Y. Wakisaka, Y. Niwa, H. Uehara, T. Ohba, S. Nozawa, K. Ichiyangai, R. Hukaya, T. Sato, S. Adachi, H. Ariga, S. Takakusagi, T. Yokoyama, B. Ohtani, K. Asakura
370. μ SR study on isolated hydrogen and oxygen vacancy in oxides. **k. shimomura**, H. Ariga, K. Asakura, E. Torikai, K. Nagamine
371. μ SR measurements of photocatalyst rutile TiO₂ single crystal. **H. Ariga***, K. Shimomura, D. Kido, A. Pant, E. Torikai, K. Nagamine, K. Asakura
372. Recent developments of positron diffraction experiment stations for surface sciences at KEK-IMSS-SPF. **K. Wada**, M. Maekawa, Y. Fukaura, I. Mochizuki, A. Kawasuso, T. Shirasawa, M. Fujinami, T. Takahashi, T. Shidara, T. Hyodo
373. Total-reflection high-energy positron diffraction (TRHEPD) analysis for the determination of rutile-TiO₂(110)-(1×2) surface structure. **I. Mochizuki***, H. Ariga, Y. Fukaura, K. Wada, M. Maekawa, A. Kawasuso, K. Asakura, T. Shidara, A. Ichimiya, T. Hyodo
374. Polarization dependent total reflection fluorescence (PTRF)-XAFS study of atomically dispersed metals on a TiO₂(110) surface premodified with mercaptobenzoic acid molecules. **S. Takakusagi***, H. Nojima, A. Kunimoto, K. Miyazaki, H. Ariga, H. Uehara, W. Chun, Y. Iwasawa, K. Asakura
375. NEXAFS and soft X-ray photoelectron spectroscopy studies on ordered V oxide films on Ag(100). **K. Edamoto***, T. Nakamura, Y. Sugizaki, K. Ozawa
376. Development of surface sensitive XAFS method based on Kramers-Kronig relations for surface chemistry. **H. Abe***, Y. Niwa, H. Nitani, M. Nomura
377. Structural investigation of supported Co oxide nanocluster catalyst using XAFS and XPS. **N. Ichikuni***, T. Fujii, H. Okuno, Y. Inoue, K. Nakajima, M. Hara, T. Hara, S. Shimizu
378. Multiscale simulation for nanomaterials and comparison with synchrotron radiation results. **Y. Li**
379. Local atomic structure of fission products in the SiC layer of irradiated TRISO fuel particles. **R.L. Seibert***, D. Velazquez, J. Terry, K. Terrani
380. Crystallization process of biomimetically deposited hydroxyapatite on TiO₂ nanotubes. **L. Liu***, S. Kim, X. Guo, J. Li, P. Shen, T.K. Sham
381. Preparation and hydrogenation activity of SBA-15 supported nanosized niobium carbide catalyst. **F. Yanagase***, N. Ichikuni*, K. Mitsuhasha, T. Hara, S. Shimizu
382. Multi-points XAFS analysis of the Pd/Al₂O₃ catalyst overlayer in an actual degraded micro gas sensor. **T. Wada***, N. Murata, T. Suzuki, H. Uehara, H. Nitani, Y. Niwa, M. Uo, K. Asakura
383. EXAFS applications to the model fuel cell catalyst. **K. Asakura**

Hawaii Convention Center
Halls I, II, III

Frontiers of Photon Upconversion Based on Triplet-triplet Annihilation (#420)

Organized by: P. Zhang, Y. Murakami, J. Zhao
Presiding: Y. Murakami, P. Zhang, J. Zhao

- Poster Session
10:00 – 12:00

- 384.** Plasmon-enhanced homogeneous and heterogeneous triplet-triplet annihilation by gold nanoparticles. **X. Cao**, B. Hu, R. Ding, P. Zhang*

- 385.** Aggregation-free doping of donor in solid acceptor arrays for low-power photon upconversion. **M. Hosoyamada**, N. Yanai, N. Kimizuka*

- 386.** Photon upconversion in air-saturated water based on amphiphilic self-assembled assembly of chromophores. **H. Kouno**, N. Yanai, N. Kimizuka*

- 387.** Columnar liquid crystals for low-power photon upconversion. **K. Mase**, N. Yanai, G. Watanabe, A. Monguzzi, N. Kimizuka*

- 388.** Air-stable and highly efficient photon upconversion in self-assembled molecular systems. **T. Ogawa**, N. Yanai, N. Kimizuka*
- 389.** Triplet-triplet-annihilation-based up-converted light from microcrystalline solid. **Y. Sakagami**, K. Kamada

Hawaii Convention Center
310 Theatre

Frontiers of Plasmon Enhanced Spectroscopy (#428)

Organized by: Y. Ozaki, Z. Tian, B. Ren, N. Halas, A. Brolo, T. Itoh, M. Moskovits
Presiding: M. Moskovits, G.C. Schatz

- 8:00 – 390.** Plasmon-enhanced properties of molecules near and far from gold nanorods. **C. Murphy***

- 8:20 – 391.** Probing different plasmonic modes of Au nanoclusters coupled to Au mirror systems with SERS. **L. Tay**, J. Hulse, J. Fraser

- 8:40 – 392.** Exploring the effect of intermolecular H-bond and the application in enantioselective discrimination by SERS. Y. Wang*, W. Ji*, Y. Ozaki*, B. Zhao*

- 9:00 – 393.** Surface enhanced Raman spectroscopy of molecular adsorbates on atomically defined surface sites. **K. Ikeda***

- 9:20 – 394.** Lighting up the Raman signal of molecules in the vicinity of graphene related materials. **J. ZHANG**

- 9:40 – 395.** Surface-enhanced Raman sensing through mesopores. **C.L. Haynes**, Z. Gao, A. Campos

- 10:00 – 396.** Combined one- and two-photon NIR excited surface enhanced Raman scattering for bio-applications. **J. Kneipp***, Z. Heiner, M. Gühlike, F. Madzarova, T. Büchner, D. Drescher

- 10:20 – 397.** Monitoring PT-103 interactions with DNA by means of AFM, TERS, SERS, ATR-FTIR, resonant inelastic X-ray scattering, and nano-IR. **B.R. Wood**, E. Lipiec, W. Kwiatek, G. Deacon, J. Sa, A. Kulik, Y. Kayser, J. Szlachetko, P. Haputhantri, D. McNaughton

- 10:40 – 398.** Plasmon-mediated biosensing of glycan expression on positionally-controlled single cells. M. Tabatabaei, G. Wallace, F. Lagugné-Labarthet*

- 10:55 – 399.** Giant enhancement of the Raman intensity due to 1D ZnO nanostructures. **S. Yoon***, H. Shin, T. Nguyen, H. Moon, J. Park, Y. Choi

- 11:10 – 400.** Nanoscale characterization of local structure on epitaxial graphene using tip-enhanced Raman spectroscopy. **S. Vantasin**, Y. Tanaka, T. Suzuki, T. Itoh, Y. Kutuma, T. Kaneko, Y. Ozaki*

- 11:25 – 401.** Isomerization of a single molecule on an STM tip. **L. Rios**, N. Tallarda, J. Lee, V.A. Apkarian*

* Principle Author

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11:40 – 402. High-sensitive molecular detection by metamaterial infrared absorber.
T. Tanaka*, A. Ishikawa

Hawaii Convention Center
307AB

Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)

Organized by: H. Sekiya, T. Zwier,
M. Fujii, E. Bieske, N. Kim
Presiding: E. Bieske, M. Fujii

8:00 – 403. Isolating the spectral signature of H_3O^+ in the smallest droplet of dissociated HCl acid. **J. Bowman***, J. Mancini , R. Conte, C. Qu

8:20 – 404. Rydberg series of alkali atoms on helium nanodroplets: Probing the screening effects of a nanosized helium dielectric. **F. Lackner***, W.E. Ernst

8:40 – 405. Angle-resolved photoelectron spectroscopy of nanosized aerosol particles. **R. Signoril***

9:05 – 406. Ion hydration in aqueous nanodrops. **E. Williams**, R. Cooper, M. DiTucci

9:30 – 407. Time-resolved radiation chemistry: Electron dynamics in iodide-nucleobase clusters. **D. Neumark***

9:55 Break

10:10 – 408. Vibrational spectra and structures of silicon hydride cluster cations. **O. Dopfer***

10:35 – 409. Assessing internal energy in gas-phase cluster ions: Measurement, modeling, and structural effects. **J. Lisy***

11:00 – 410. Drastic changes in IR spectral features of solvated metal ions caused by rare-gas attachment. **K. Ohashi***, H. Sekiya

11:20 – 411. Novel double-resonance laser spectroscopy technique in a cold quadrupole ion trap and its application to protonated adenine dimer. **H. Kang***

11:40 – 412. Effective molecular model for gas phase spectroscopy of short-lived biomolecules: Application to IR spectroscopy and anharmonic vibrational calculation. **H. Asami***, M. Tokugawa, Y. MASAHI, E. GLOAGUEN, K. SEIO, H. Saigusa, M. Sekine, Ch. Mons

Hawaii Convention Center
306A

Interplay between Chemistry and Dynamics in Biomolecular Machines (#441)

Organized by: S. Hayashi, A. Kitao, Y. Rhee, E. Tajkhorshid
Presiding: E. Tajkhorshid

8:00 Opening Remarks

8:05 – 413. Structural dynamics of biomolecular machines filmed with time-resolved X-ray lildography and crystallography. **H. Ihie***

8:35 – 414. Interplay between chemistry and dynamics in a photon manufacturing protein-chromophore complex. **Y. Rhee**

9:05 – 415. Crucial role of protein flexibility in enzymatic catalysis. **S. Hayashi***

9:35 – 416. Efficient fluorescence emitter and the biomolecular environment: Understanding the photodynamics of the fluorescent protein with computer simulations. **J. Park***

9:55 Break

10:10 – 417. Coupling of mesoscale biomolecular phenomena to ATP hydrolysis. **G. Voth**

10:40 – 418. Dynamics of linear and rotary molecular motors revealed by gold nanoprobes. **R. Iino***

11:10 – 419. Mechanochemical coupling and information fidelity control in simple biomolecular machinery. **J. Yu***

Wednesday Afternoon

Hawaii Convention Center
308A

Ultrafast Intense Laser Chemistry (#35)

Organized by: K. Yamanouchi, R. Lewis, F. Legare, Q. Gong
Presiding: K. Yamanouchi

13:00 – 420. Revealing phase structure of strong-field molecular tunneling wave packets. **Y. Liu**

13:25 – 421. Nonadiabatic tunnel ionization of atomic and molecular degenerate orbitals in strong circularly polarized laser fields. **I. Barth**, J. Berakdar, M. Lein, K. Liu, O. Smirnova

13:40 – 422. Electron currents in vibrating H_2^+ . **K. Renziehausen**, I. Barth*

13:55 – 423. Laser-polarization dependence of atomic/molecular multiphoton excitation with a single-active-electron model of spherical symmetry. **M. Kanno**, N. Inada, H. Kono*

14:10 – 424. Decomposition of the configuration-interaction coefficients in the multi-configuration time-dependent Hartree-Fock method. **E.V. Lotstedt***, T. Kato, K. Yamanouchi

14:25 Break

14:40 – 425. Characterization of the carrier envelope phase of an isolated attosecond pulse. **F. He***

15:05 – 426. Determination of absolute CEP of circularly-polarized few-cycle laser pulses by angle-resolved photoelectron spectra of tunnel-ionized photoelectrons. **S. Fukahori***, T. Ando, S. Miura, R. Kanya, K. Yamanouchi, T. Rathje, G.G. Paulus

15:20 – 427. Ultrafast light manipulation using molecular and metallic nanostructures. **Q. Gong***, H. Yang*, J. Chen, X. Hu

15:45 – 428. Table-top water window ultrafast X-ray source and applications. **F. Légaré**, B.E. Schmidt, N. Thiré, S. Beaulieu, V. Cardin, V. Wanlie, F. Sylvain, J. Kieffer, M. Negro, C. Vozi

16:10 Closing Remarks

Hawaii Convention Center
308B

New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems (#84)

Organized by: T. Carrington, J. Bowman, D. Zhang
Presiding: R.B. Shirts

13:00 – 429. Using diffusion Monte Carlo to explore the spectroscopy and dynamics of molecules and ions that undergo large amplitude vibrational motions. **A.B. McCoy***, M. Marlett, Z. Lin

13:30 – 430. Permutation invariant polynomial-neural network (PIP-NN) approach to multidimensional potential energy surfaces for gas phase and gas-surface systems. **G. Guo**

14:00 – 431. High dimensional quantum dynamics studies of chemisorption of polyatomic molecules on metal surfaces. **D. Zhang***

14:30 – 432. On-the-fly ab initio semiclassical dynamics for computing vibrationally resolved electronic spectra. **M. Wehrle, M. Sulc, S. Oberli, J. Vanicek**

15:00 Break

15:20 – 433. Role of the intermolecular interactions on high pressure transitions in $\text{Ar}-\text{H}_2\text{O}$ clusters. **D.J. Arismendi Arrieta**, A. Vitek, R. Rodriguez-Cantano, R. Kalus, R. Prosmits, P. Villarreal, G. Delgado-Barrio

15:40 – 434. Computational spectroscopy and thermodynamics of small clusters of atmospheric interest. **L. Halonen***

16:10 – 435. Theoretical study of the internal conversion from S_1 to S_0 in H_2CO : Effects on dynamics when including the second derivative terms of nonadiabatic coupling matrix elements. **T. Nakajima**

16:30 – 436. Small molecules in nanocavities: Translation-rotation eigenstates, spectra, and new selection rules from multidimensional quantum calculations. **Z. Bacic***, M. Xu, S. Ye, A. Powers

Hawaii Convention Center
305B

Deciphering Molecular Complexity from Single Molecules to Cellular Networks (#121)

Organized by: T. Komatsuzaki, J. Wang, J. Wu
Presiding: M. Sasai, J. Wang

13:00 – 437. Genetic network underlying the epithelial-mesenchymal transition (EMT). **H. Levine***

13:35 – 438. Acetate overflow: Optimal proteome partitioning and regulation. **X. Li***, L. Tang*

14:05 – 439. Let there be force: Modeling cell-ECM interactions in cancer invasion. **Y. Jiang***

14:35 Break

14:50 – 440. Decision making at the cell level: From bacteria to possibly cancer. **J.N. Onuchic**

15:25 – 441. Single-molecule imaging for systems biology via quantum metrology. **F. Herrera***

15:40 – 442. Pathways and networks: Unraveling the complex organization of signaling networks. **A. Levechenko***

16:10 – 443. Landscape and fluxes of neural networks. **J. Wang***

16:40 Closing Remarks

Hawaii Convention Center
305A

Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130)

Organized by: A. Wilson, P. Schwerdtfeger, K. Kim, Z. Lin, T. Cundari
Presiding: N.J. DeYonker

13:00 – 444. Helical gold nanorods and related gold nanostructures. **I.P. Hamilton***, X. Liu*

13:30 – 445. Thiolene or thiolate: Their non-innocent nature in transition metal complexes. **M. Hall**, H. Li, H. Tang

14:00 – 446. Electronic interactions between two transition-metal termini through carbon bridges: What can DFT say (or cannot say)? **J. Halet***

14:30 BREAK

14:45 – 447. Efficient description of electron correlation effects in actinide compounds. **P. Tecmer**, K. Boguslawski, P. Ayers

15:15 – 448. Theoretical analysis in probing factors influencing metal-metal bond strength. **M.B. Pastor**, Q. Zhao

15:45 – 449. Changing the nature of agnostic and agostic interactions - a synthesis by computation approach. **A. Nielson***, J. Harrison, A. Sajjad, P. Schwerdtfeger

16:05 – 450. Accurate two-component relativistic theory based on local unitary transformation and frozen potential schemes for large molecules including heavy elements. **J. Seino***, Y. Nakajima, H. Nakai

16:25 – 451. X-ray spectra of iron complexes: A challenge for quantum chemistry. **A.J. Atkins, J. Rudolph, M. Bauer, C.R. Jacob**

Hawaii Convention Center
306B

Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134)

Organized by: P. Piotrowiak, M. Fujii, J. Tang, B. Zhang
Presiding: M. Fujii, J. Papanikolas

13:00 Introductory remarks

13:05 – 452. Extending decades-old chemistry and physics to improve modern molecular imaging. **W.S. Warren***

13:45 – 453. Cooperative singlet and triplet exciton transport inorganic semiconductors visualized by ultrafast microscopy. **L. Huang***

14:15 – 454. Using pump-probe microscopy to visualize charge carrier dynamics in semiconductor nanowires. **J. Papanikolas***

14:45 Break

15:00 – 455. Vibrational imaging by two-color infrared microscope. **M. Fujii***, M. Sakai

15:30 – 456. kHz frame-rate multichannel beam-scanning microscopy based on Lissajous trajectories. **S. Sullivan**, j. Newman, R. Muir, M. Carlsen, s. sreehari, C. Bouman, **G.J. Simpson***

16:00 – 457. In situ measurement of adlayer growth and adlayer hydration on metal nanoparticles by photothermal microscopy. **E. Koh**, I.B. Tsvetkova, B. Dragnea

16:30 – 458. Kerr-gated fluorescence microscopy of P3HT on nanostructured gold and silver. **P. Piotrowiak**, J. Bao, L. Gundlach, D. O'Carroll, Z. Yu

Hawaii Convention Center
313C

Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)

Organized by: J. Hasegawa, M. Collins, M. Gordon, P. Piecuch, T. Taketsugu
Presiding: M.S. Gordon

13:00 – 459. Photoinduced proton-coupled electron transfer in solution: Quantum mechanical/molecular mechanical non-adiabatic dynamics. **S. Hammes-Schiffer**

13:30 – 460. OM/MM studies of excited states in complex systems. **S. Matsika***

14:00 – 461. Modeling intra- and inter-molecular interactions in chromophore - protein complexes for efficient photodynamic simulations. **Y. Rhee**

14:30 – 462. Automatic rhodopsin modeling as a prospective tool for high throughput photobiology. **M. Olivucci***

15:00 – 463. Theoretical study on photobiological systems. **X. Li**

15:20 – 464. On the nature of a large Stokes shift in pMIP fluorescent protein. **S. Faraji***, A. Krylov

15:40 – 465. Theoretical study on the mechanisms of the selective fluorescence of PicoGreen. **M. Okoshi**, P. Saparpakorn, Y. Takada, S. Hannongbua, H. Nakai*

16:00 – 466. Intra and intermolecular charge-transfer: Toward the control of excited state properties of molecules and materials. **A. Painelli**, C. Sissa, F. Di Maio, F. Delchiaro, S. Sanyal, F. Terenziani

16:20 – 467. Charge-transfer and local excitations in organic dyes. **C. Sissa***, V. Calabrese, M. Cavazzini, L. Grisanti, F. Terenziani, S. Quici, A. Painelli

16:40 – 468. Ground and excited state electronic structures and optical response properties of open-shell quinoidal oligothiophenes. **R. Kishi***, M. Saito, N. Matsushita, M. NAKANO

* Principle Author

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Hawaii Convention Center
313A

Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168)

Organized by: A. Terasaki, S. Anderson, N. Gaston
Presiding: A. Terasaki

13:00 – 469. Geometrical structures and reactions of metal oxide cluster ions studied by ion mobility-mass spectrometry.
K. Ohshima, R. Moriyama, J.W. Wu, N. Nomisawa, T. Komukai, S. Azuma, R. Sato, M. Latif, M. Nakano, **F. Misra***

13:30 – 470. Dispersion interactions between metal atom clusters. R. Hatz, V. Hänninen, **L. Halonen***

13:50 – 471. Reactions between series of heavy metal clusters ($\text{Ag}_n^{+/-}$, $\text{Au}_n^{+/-}$, $\text{Pb}_n^{+/-}$ and $\text{Bi}_n^{+/-}$) and O_2 . **X. Xing***, J. Ma, X. Cao

14:10 – 472. Studies on reactions of molecules on metal clusters: Approach from cluster-cluster collisions. **M. Ichihashi***, S. Hirabayashi, H. Odaka

14:30 – 473. Interfacial charge transfer and reactivity of supported metal oxide nano-clusters. M. Nakayama, M. Xue, W. An, P. Liu, **M. White***

15:00 break

15:15 – 474. Supported metallic and bimetallic nanocatalysts. **F. Baleotto***

15:45 – 475. Size-dependent correlations between supported cluster physical and catalytic properties. E. Baxter, A. von Weber, Y. Dai, T. Gorey, **S.L. Anderson***

16:05 – 476. Theoretical study of the dehydrogenation of isopropanol on Ni_{13} cluster supported on $\Theta\text{-Al}_2\text{O}_3$ surface.
A. Lyalin, K. Shimizu, T. Taketsugu

16:25 – 477. Cluster-based functional materials: Size-dependent performance of subnanometer clusters in heterogeneous catalysis, electrocatalysis, and Li-air batteries. **S. Vajda**

16:55 Closing remarks

Hawaii Convention Center
304B

Latest Development of Advanced Vibrational Spectroscopy (#187)

Organized by: K. Iwata, S. Asher, D. Phillips, Y. Furukawa
Presiding: T.L. Gustafson, K. Iwata

13:00 – 478. Reading molecular fingerprints more wisely. M. Ando, S. Yabumoto, **H. Hamaguchi**

13:25 – 479. Vibrational coherence spectroscopy as a measure of heme ruffling in cytochrome c. **P. Champion***

13:50 – 480. Probing the core and the surface of amyloid fibrils by means of Raman spectroscopy. **I.K. Lednev***, V. Sereda

14:15 – 481. Advances in the VCD study of protein amyloid fibrils. **L.A. Nafie***, R.K. Dukor, I.K. Lednev, D. Kurouski

14:40 – 482. Quantum-mechanical strategies for the calculation of vibrational optical activity spectra of complex systems. **C. Cappelli***

15:00 break

15:10 – 483. Out-of-plane hydration and conformation effects on the vibrational properties of the peptide group. **H. Torii***

15:35 – 484. Development and application of computationally-guided resonance Raman spectroscopy to investigate metallo-enzyme intermediates. **H.S. Shafaat***, P. Maugeri, A. Manesis, J. Slater, N. Trivelas, S. Behrnke

15:55 – 485. Using $^{13}\text{C} = ^{18}\text{O} / ^{15}\text{N}$ isotope dependence of the amide-I/II 2D IR cross peaks to distinguish between peptide conformations. H. Maekawa, G. Ballano, F. Formaggio, C. Toniolo, **N. Ge***

16:15 – 486. Vibrational spectroscopy of Southern Ocean phytoplankton: A new approach for understanding drivers of primary productivity. **P. Heraud***, O. Sackett, K. Petrou, J. Beardall

16:40 – 487. DNA conformation and the ultrafine structure of nuclear material in functional and fixed avian erythrocytes analysed with synchrotron FTIR and soft X-ray tomography. **B.R. Wood**, D. Whelan, D. Parkinson, J. Zhang, P. Heraud, D. McNaughton

Hawaii Convention Center
313B

Single-molecule Fluorescence Imaging (#208)

Organized by: P. Chen, T. Majima, G. Cosa
Presiding: R.H. Goldsmith, H. Lu

13:00 Frontiers of methodology II

13:00 – 488. FLUOROCODE, a super-resolution optical map of DNA. **J. Hofkens**, V. Leen

13:25 – 489. Probing neuronal receptor ion channel dynamics in living cells by a novel single-molecule patch-clamp FRET microscopy. **H. Lu***, D. Sasmal

13:50 – 490. Obtaining resolution enhanced fluorescence images and 3D orientation information of single molecules by polarization modulation. **L.S. Jess**, D. Pfennig, M. Grunwald, A. Albrecht, N. Hafi, P.J. Walla*

14:05 – 491. Development of new fluorescent sphingomyelin analogs revealed transient sphingomyelin residency in raft domains for <50 ms. **M. Kinoshita***, N. Matsumori, M. Takada, H. Ano, M. Murata, K. Suzuki, A. Kusumi

14:20 Break

14:35 Conjugated materials

14:35 – 492. Spectroscopy of single conjugated polymers and aggregates: The role of interchain and intrachain interactions. **D.A. Vanden Bout**

15:00 – 493. Structure-property relationship of macrocyclic porphyrin arrays probed by single-molecule defocused wide-field imaging. **D. Kim**

15:25 – 494. Molecular mesoscopes: A bottom-up view of organic electronics. **J.M. Lupton**

15:50 – 495. Molecular-level study and control of conformation and photophysics in conjugated molecular complexes. **M. Vacha**

16:15 – 496. What to do when (the fluorescent) lights go out: Spectroscopy of individual non-emissive doped conjugated polymers using optical microresonators. **R.H. Goldsmith***

16:40 – 497. Optical nanoimaging for block copolymer self-assemblies. **M. Zhu**

Hawaii Convention Center
301A

Fundamental Science of Photon and Electron Induced Surface Processes (#228)

Organized by: H. Petek, J. Zhao, Y. Matsumoto
Presiding: U. Höfer

13:00 Introductory remarks

13:05 – 498. Model systems in catalysis for energy economy. **H. Freund***

13:45 – 499. Controlling the transport and reaction of hydrogen at Pd(110) and $\text{Pd}_2\text{Au}_{30}(110)$ surfaces. **K. Fukutani**, S. Ohno, S. Ogura, M. Wilde

14:25 – 500. Observing and manipulating individual NH molecules and H atoms on the Pt(111) surface. Z. Liang, H. Yang, J. Oh, Y. Kim, **M. Trenary***

14:45 Coffee break

15:00 – 501. CO_2 capture by 1D self-assembled surface metal-organic frameworks at the molecular scale. **M. Feng**

15:20 – 502. Substrate-induced control of molecular motion at a metal surface. **L. Bartels**

16:20 – 503. Coherent phonons of Cs intercalated graphene on Ir(111).

K. Watanabe, M. Petrović, M. Kralj, P. Lazic, T. Sugimoto, Y. Matsumoto*

16:40 – 504. Plasmon-phonon dynamics at Ga/Pt/Si(001) interfaces. **K. Ishioka***, K. Brixius, A. Beyer, W. Stoltz, K. Volz, U. Höfer, H. Petek

Hawaii Convention Center
312

Interplay between Theory and Experiment in Catalytic Research (#277)

Organized by: M. Ehara, C. Cramer, S. Dai, C. Jones, T. Ziegler, T. Tsukuda

13:00 – 505. Theoretical studies on the bond activation in heterogeneous catalysis. **M. Ehara***

13:20 – 506. Enhanced catalysis with nano confinement. **X. Bao**

13:45 – 507. Addressing selectivity challenges in heterogeneous catalysis: Formic acid decomposition on transition metals. **M. Mavrikakis***, J.A. Dumesic, J. Scarcato, S. Li, S. Singh, S. Ranganajan, J. Herron, L. Roling, R. Carrasquillo, B. O'Neill

14:10 – 508. Electrocatalytic oxygen reduction using atomic platinum catalysts dispersed on titanium nitride. **H. Lee***, S. Yang, A. Soon

14:25 – 509. Rate enhancement and low temperature activation for C-C coupling of carboxylic acids with dilute Co incorporation in MFI. **J.C. Hicks***

14:40 – 510. Hydrogen production from formic acid as an energy storage materials using Pd and Pd alloy catalysts. **K. Mori**, M. Dojo, H. Yamashita

14:55 Break

15:10 – 511. Utility of new generations of coupled-cluster methods and algorithms in catalytic, structural, and optical properties of gold nanoparticles. **P. Piecuch***, J.A. Hansen, N.P. Bauman, M. Ehara

15:35 – 512. Catalyst development for the realization of carbon-neutral energy cycles. **M. Yamauchi***

16:00 – 513. Mechanistic investigation of highly robust hydrogen generation by new bioinspired Ir complexes for dehydrogenation of formic acid in water. **M.Z. Ertem**, W. Wang, Y. Himedha, E. Fujita, T.J. Muckerman

16:15 – 514. Understanding and design of organometallic reactivity with experimental and computational tools. **F. Schoenebeck***

16:30 – 515. Theoretical investigation of catalytic activity of boron nitride based nanomaterials for oxygen reduction reaction and interplay with experiment.

T. Taketsugu*, A. Lyalin, A. Nakayama, G. Elumalai, H. Noguchi, T. Masuda, K. Uosaki

16:45 – 516. Rational design of the catalysts for heterogeneous hydrogenation of amides to amines. **X. Cao***, P. Hu

Hawaii Convention Center
301B

Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370)

Organized by: W. Zhao, W. Zhuang,

M. Cho, G. Sholes

Presiding: M. Cho

13:00 – 517. Dynamics in the isotropic phase of liquid crystals. **M.D. Fayer***, K.P. Sokolowsky, H.E. Bailey

13:25 – 518. Broadband 2D UV studies of DNA: Challenging concepts of inherent photostability of genetic material.

R. Miller*, H. Duan, S. Maneshi, P. Nalbach, A. Picchietti, M. Pola, V. Prokhorenko, A. Stevens, M. Thorwart

13:50 – 519. Extending multidimensional concepts of heterogeneity to single-molecule spectroscopy and solvation dynamics. S. Verma, H. Wu, **M.A. Berg***

14:15 – 520. Ultrafast vibrational spectroscopy of electronic processes in solution processed photovoltaic materials. **J. Asbury***

14:40 – 521. Intermolecular vibrational energy transfers in liquids: Phonon-compensation or dephasing?. **J. Zheng**

15:20 Break

15:20 – 522. Verification of the vibronic origin of long-lived coherence in an artificial molecular light harvester. **J. Hauer***

15:45 – 523. 2D-IR spectroscopy of strongly coupled hydrogen-bonded complexes. A.M. Stingle, B.L. Van Hoozen, **P. Petersen**

16:10 – 524. Mapping the vibronic structure and dynamics of complex systems by single-shot supercontinuum 2D spectroscopy. **E. Harel***

16:30 – 525. Dynamics of protein molecular recognition via 2D IR spectroscopy. R. Horness, E. Basom, A. LeSueur, **M. Thielges***

Hawaii Convention Center
310 Theatre

Frontiers of Plasmon Enhanced Spectroscopy (#428)

Organized by: Y. Ozaki, Z. Tian, B. Ren, N. Halas, A. Brolo, T. Itoh, M. Moskovits
Presiding: A.G. Brolo, B. Ren

13:00 – 526. Plasmonically coupled nanostructures and their biomedical applications. **J. Nam***

13:20 – 527. Distinguishing different molecules at the nanoscale by plasmon enhanced Raman scattering. **Z. Dong**

13:40 – 528. Current understanding of lateral and spatial resolution in tip-enhanced Raman scattering. **V. Deckert***

14:10 – 529. Infrared nanoscopy and nanospectroscopy – from vibrational spectroscopy to plasmon mapping. **R. Hillenbrand**

14:30 – 530. Toward extreme spatial and temporal resolution by tip enhanced spectroscopy in ambient. **N. Hayakawa***

14:50 Break

15:05 – 531. Plasmonic arrays. **G.C. Schatz**

15:35 – 532. Chemical reactions on plasmonic nanostructures. **H. Xu***

15:55 – 533. Measuring the enhanced and modified absorbance of molecules adsorbed to metallic nanostructures. **B. Darby***, M. Meyer, B. Auguie, E. Le Ru

16:10 – 534. Wavelength dependent energy transfer and metal-enhanced fluorescence. **Y. Pang**, J. Lee, M. Jen, S. Lee

16:25 – 535. Blinking from multicolored SERS-active Ag nanoaggregates. **Y. Kitahama***, T. Nagahiro, Y. Tanaka, T. Itoh, Y. Ozaki

16:40 – 536. Theoretical methods for infrared absorption spectroscopy with non-uniform electric fields. **T. Iwasa***, T. Taketsugu

Hawaii Convention Center
307AB

Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)

Organized by: H. Sekiya, T. Zwier, M. Fujii, E. Bieske, N. Kim
Presiding: N. Kim, T.S. Zwier

* Principle Author

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- 13:00 – 537.** Potential energy surfaces and the reaction dynamics of excited-state multiple proton transfer in the 7-azaindole complexes and the role of mediating alcohols. **Y. Kim***
- 13:25 – 538.** Spectroscopic features of molecular aggregates from anharmonic computations. **M. Biczysko***, T. Fornaro, J. Bloino
- 13:45 – 539.** Selenium centered hydrogen bonding (SeCl_2H) interaction. **S. Chakraborty***
- 14:05 – 540.** Positively charged phosphorus as a hydrogen bond acceptor. **A. Hansen**, L. Du, H.G. Kjaergaard
- 14:25 – 541.** Structural motifs of aqueous clusters: Insights from the modeling of their infrared spectra obtained from high-levels of electronic structure theory. **S.S. Xantheas***
- 14:50** Break
- 15:05 – 542.** Frequency- and time-domain investigation on intermolecular vibrations of molecular clusters. **Y. Ohshima**
- 15:30 – 543.** Imaging bond breaking and vibrational energy transfer in water containing clusters. **H. Reisler***
- 15:55 – 544.** Experimental and theoretical study on the excited state dynamics of methyl cinnamate and its derivatives. **T. Ebata***, Y. Inokuchi, Y. Miyazaki, N. Akai
- 16:20 – 545.** Molecular level inspection of H-bond rearrangement and fluctuation in the gas phase. **K. Sakota***
- 16:40 – 546.** Real-time observation of photoionization-induced water migration in 5-hydroxyindole-water cluster. **A. Naito**, M. Miyazaki, T. Imajyo, H. Sekiya, M. Fujii

Hawaii Convention Center
306A

Interplay between Chemistry and Dynamics in Biomolecular Machines (#441)

- Organized by:* S. Hayashi, A. Kitada, Y. Rhee, E. Tajkhorshid
Presiding: Y. Rhee
- 13:00 – 547.** Millisecond dynamics of RNA polymerase II translocation at atomic resolution. **X. Huang***
- 13:30 – 548.** Ribosomes in motion: The dynamics of nature's protein synthesis machinery. **R.L. Gonzalez, Jr.***
- 14:00 – 549.** Simulating conformational changes of the ribosome. **K. Sanbonmatsu**
- 14:30 – 550.** Computational study on flexible dynamics of histone tails. **S. Fuchigami***
- 14:50** Break
- 15:05 – 551.** Mechanism of transmembrane voltage-sensing in voltage-dependent potassium ion and proton channels. **D. Tobias***
- 15:35 – 552.** Dielectric constant and water penetration gradients along transmembrane peptide-lipid bilayer interface. **T. Smirnova***, M. Voynov, A. Srinivas
- 15:55 – 553.** Permeation, gating, and modulation of voltage-gated potassium channels. **M.O. Jensen***
- 16:25 – 554.** Characterizing large-scale conformational transitions in membrane transporters at high spatial and temporal resolutions. **E. Tajkhorshid**

Wednesday Evening

Hawaii Convention Center
Halls I, II, III

Ultrafast Intense Laser Chemistry (#35)

- Organized by:* K. Yamanouchi, R. Lewis, F. Legare, Q. Gong
Presiding: K. Yamanouchi
- Poster Session**
19:00 – 21:00
- 555.** Direct time-resolved spectroscopy studies of the photoreactions of antifungal and photosensitizing drug itraconazole. **R. Zhu***, M. Li, D.L. Phillips
- 556.** Field-free orientation dynamics of OCS molecules induced by a pre-alignment method. **K. Sonoda***, T. Sato, A. Iwasaki, K. Yamanouchi, H. Hasegawa

- 557.** Ultrafast dynamics of photoexcited electrons and coherent phonons in the topological insulator. **K. NORIMATSU**, M. Hada, S. Tanaka, K. Igashiri, T. Ishikawa, K. Onoda, T. Sasagawa, K.G. Nakamura
- 558.** Time-resolved X-ray absorption spectroscopy (TR-XAS) study on the metal-to-ligand charge-transfer (MLCT) states of $\text{Ru}(\text{bpy})_2(\text{dppp})^{2+}$. **R. Ma**, T. Kim*

Hawaii Convention Center
301B

Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60)

- Organized by:* A. Kovalenko, B. Pettitt, F. Hirata
Presiding: A. Kovalenko, M. Pettitt
- 19:00 – 559.** Solvation-induced self-assembly of polyelectrolyte membranes. **A.V. Neimark***, A. Vishnyakov, M. Lee
- 19:30 – 560.** Molecular multipole models for water. **T. Ichijo***
- 20:00 – 561.** Extension of COSMO-RS to phase boundaries, micelles, and biomembranes. **A. Klamt**

Hawaii Convention Center
Halls I, II, III

New Insights from Quantum Dynamics and ab initio Potentials in High Dimensional Systems (#64)

- Organized by:* T. Carrington, J. Bowman, D. Zhang
Presiding: D. Babkov

Poster Session

19:00 – 21:00

- 562.** First-principles and tight-binding quantum chemical molecular dynamics simulations on low friction mechanism of carbon nitride thin films. **M. Nakamura**, S. Sato, H. Murabayashi, T. Tsuruda, Y. Wang, S. Bai, Y. Higuchi, N. Ozawa, K. Adachi, M. Kubo*

Hawaii Convention Center
Halls I, II, III

Computational Modeling of d- and f-Block Chemistry: Challenges and Opportunities (#130)

- Organized by:* A. Wilson, P. Schwerdtfeger, K. Kim, Z. Lin, T. Cundari
Presiding: K.S. Kim

Poster Session

19:00 – 21:00

- 563.** Cooperation in bi-/multi-nuclear metal complexes: Insights from computational studies. G. Luo, X. Kang, Z. Hou, **Y. Luo***
- 564.** Theoretical study of the interaction of carbon dioxide with the $[\text{VCl}(\text{MesO})_2(\text{THF})_2]$ complex. **W.D. Quintero Martinez***, I. Ortíz Verano*
- 565.** Ground and low-lying excited states of PtCN and PdCN: Theoretical investigation including spin-orbit coupling. **J. Moon**, J. Kim

- 566.** First-principles prediction of X-ray photoelectron spectra beyond DFT. **N.D. Keilbart**, N. Poilvert, I. Dabo

- 567.** Electronic structure in lanthanum and cerium salen complexes. **C.E. Gaitan Caicedo***, I. Ortíz Verano*
- 568.** 3D visualization of relativistic wave functions for intuitive understanding of electronic structure. **K. Ogasawara***

Hawaii Convention Center
Halls I, II, III

Chemical Imaging: Frontiers of Spatio-Temporal Resolution (#134)

- Organized by:* P. Piotrowiak, M. Fujii, J. Tang, B. Zhang

Poster Session

19:00 – 21:00

- 569.** Orientation-sensitive IR imaging of feather β -keratins by a VSFG-detected IR super-resolution microscopy. **Y. Watase***, K. Ushio, M. Fujii, M. Sakai

Hawaii Convention Center
313C

Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)

- Organized by:* J. Hasegawa, M. Collins, M. Gordon, P. Piecuch, T. Taketsugu
Presiding: J. Hasegawa

- 19:00 – 570.** Excitation energy transfer and vibronic couplings in multichromophores. **L. Slipchenko**

- 19:30 – 571.** Toward quantitative analysis of excitation energy transfer in light-harvesting antennas. **M. Higashi***

- 20:00 – 572.** Excited-state dynamics at inter-system crossings in first-row transition metal complexes and clusters. **D.S. Kaliakin, R.R. Zaari, D.A. Fedorov, G.E. dePolo, A.O. Lykhin, S.A. Varganov***

- 20:20 – 573.** Real-time non-adiabatic modeling of time-resolved transient absorption and photoelectron ionization spectra of cyclohexadiene derivatives. **E. Tapavicza***, T. Thompson, N. Baluyot, W. Narvaez, O. Schalk, R.J. Sension

- 20:40 – 574.** Charge-transfer dynamics of light-harvesting systems in complex solvated environments. **B.M. Wong**, M. Oviado

Hawaii Convention Center
Halls I, II, III

Frontiers of Metal Clusters and Nanostructures: From Fundamental Properties to Functionalities (#168)

- Organized by:* A. Terasaki, S. Anderson, N. Gaston

Poster Session

19:00 – 21:00

- 575.** Systematic investigation of the superatomic character of heteroatom doped, thiolate protected gold clusters. **J. Schacht, N. Gaston**

- 576.** Understanding of ligand exchange reaction mechanism of thiolate-protected metal clusters by usage of high-resolution high-performance liquid chromatography. **Y. Nilohri**, Y. Negishi

- 577.** Influence of size and temperature on the shape preference of Au nanoparticles. **A.L. Garden**, A. Pedersen*, H. Jónsson

- 578.** Effects of the alkynyl substituents on the geometrical and electronic structures of "Magic-Number" Au_{13} cluster. **M. Sugiuchi***, Y. Shichibu, K. Konishi

- 579.** Blue luminescence of dendrimer-encapsulated gold nanoclusters. **J. Song**

- 580.** Controlling of anisotropy of porphyrin-coordinated Au cluster. **M. Sakamoto**, D. Eguchi, T. Teranishi

- 581.** Density of states analogy between Pd-metal and $\text{Ag}_{0.5}\text{Rh}_{0.5}$ alloy. **Y. Namba**, T. Ishimoto, M. Koyama

- 582.** Vibrational properties of core-shell Au_nX_m ($\text{X} = \text{Ag}$ and Pt) nanoparticles. **H.E. Saucedo***, D.A. Velasco, I.L. Garzon

- 583.** Chemical reactivity of silver-cobalt binary cluster ions: Effects of geometric and electronic structures. **S. Sarugaku**, R. Murakami, J. Matsumoto, M. Arakawa, A. Terasaki

- 584.** Electronic structures of Ag-Rh alloy nanoparticles: Size dependency and relation with hydrogen absorption. **K. Miyazaki**, A. Matsuda, H. Mori*

- 585.** Structure and photodissociation reaction of metal-acetone cluster ions $M^+(\text{CH}_3\text{COCH}_3)_n$ ($M = \text{Cu}, \text{Ti}, \text{Sm}$, and Er) studied by time-of-flight reflectron imaging spectrometry. **Y. Yamakita***, K. Saito, S. Shimokawara, H. Iwasaki

- 586.** Capturing mechanism of gas-born metal nanoparticles into solutions. **K. Omori**, **N. Sakono***

- 587.** Trapping a liquid micro-droplet in a vacuum toward wet chemistry of gas-phase clusters. **K. Ando**, M. Arakawa, A. Terasaki

- 588.** Theoretical study on hydrogen storage properties of Pd nano cluster: Consideration on cluster shape dependency. **A. Matsuda***, H. Mori

- 589.** Theoretical study of core-shell alloy of Pd and Pt interacting with hydrogen. **N. Binti Zukiffi***, T. Ishimoto, M. Koyama

- 590.** Size-effect on electrochemical water reduction by size-selected Pt nanoclusters deposited on $\text{SrTiO}_3(100)$. **Y. Yamano**, C. Zhang, R. Kobayashi, T. Eguchi, H. Tsunoyama, A. Nakajima*

- 591.** Theoretical study of stability of Pd/Pt nanoparticles. **T. Ishimoto**, M. Koyama

- 592.** First principles study of diffusion dynamics of defects in semiconductor quantum dots. **A. Petrone***, E. Cheng, D.B. Williams-Young, D. Lingertelt, X. Li

- 593.** Genuinely amorphous carbon from explosive nano copper acetylide. **K. Judai***, Y. Hatakeyama

- 594.** On the catalytic role of ligands in supported Au_nR_m nanoclusters. **Z. Wu**, D.R. Mullins, L. Allard, S.H. Overbury

- 595.** Exploration on magic nanoclusters in silicon-transition metal binary systems by reaction with molecular oxygen. **Y. Sugawara**, T. Nagase, H. Tsunoyama, A. Nakajima*

- 596.** New magnetic superatom: $\text{Cr}@\text{Zn}_{17}$. **A. Vega***, A. Aguado, A. Lebon

- 597.** Chemical evaluation of $\text{Ta}@\text{Si}_{16}$ nano-cluster deposited on graphite surface by X-ray photoelectron spectroscopy. **T. Ohta**, M. Shibuta, H. Tsunoyama, T. Eguchi, A. Nakajima*

- 598.** Pseudo-atom behavior of $M@\text{Al}_{12}X$ ($M = \text{B}, \text{C}, \text{N}, \text{Al}, \text{Si}, \text{P}$): A theoretical study. **B. Molina***, J. Soto, J. Castro

- 599.** Nano material produced by laser ablation and magnetron sputtering of metal. **K. Kitamura**, K. Judai

- 600.** Size-selected vanadium oxide clusters on $\text{TiO}_2(110)-(1\times 1)$ and their role in oxidative dehydrogenation of methanol: Every atom counts. **J.W. Buffon**, H.L. Neilson, J. Robins, S.K. Buratto*

- 601.** Photodissociation spectroscopy of silver cluster cations up to 35 atoms: Size and temperature dependence of spectral profiles. **K. Tobita**, Y. Kiyomura, T. Ito, M. Arakawa, A. Terasaki

- 602.** Reaction of cationic rhodium clusters, Rh_n^{+} , with NO in thermal energy region. **Y. Tawaraya**, S. Kudoh, K. Miyajima, F. Mafune*

- 603.** Computational study of the molecular oxygen adsorption on bimetallic $\text{Au}_n\text{Pd}_m^{+}$ cationic clusters with $n+m = 2-5$. **L.C. Balbás***

- 604.** Temperature-programmed desorption of NO adsorbed on Ir clusters. **K. Koyama**, S. Kudoh, K. Miyajima, F. Mafune*

- 605.** Reactivity of cerium oxide clusters with NO and CO revealed by temperature-programmed desorption in the gas phase. **T. Nagata**, K. Miyajima, F. Mafune*

- 606.** Reaction of size-selected silicon-oxide cluster anions with CO and H_2O as a model for chemistry on mineral surfaces. **M. Arakawa**, R. Yamane, A. Terasaki

- 607.** Desorption energy of oxygen molecule from rhodium oxide clusters probed by temperature-programmed desorption. **M. Takenouchi**, K. Miyajima, F. Mafune*

* Principle Author

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608. Release of oxygen from the palladium oxide clusters by heat. **K. Miyajima, F. Mafune***

Hawaii Convention Center
Halls I, II, III

Latest Development of Advanced Vibrational Spectroscopy (#187)

Organized by: K. Iwata, S. Asher, D. Phillips, Y. Furukawa

Poster Session

19:00 – 21:00

609. Quantum and semiclassical studies of weak adjacent substituent effect on the overtone intensities for the X(H=C,O) stretching vibrations. H. Takahashi, K. Takahashi, **S. Yabushita***

610. Vibrational SCF-CI calculations using the curvilinear coordinate. **H. Iwase, K. Hashimoto***

611. Vacuum ultraviolet mass-analyzed threshold ionization spectroscopy of oxetane. D. Kang, **H. Kim***, C. Kwon

612. Cationic structures of azabenzenes by one-photon mass-analyzed threshold ionization spectroscopy. Y. Lee, H. Kim, **C. Kwon***

613. Vibrational structure of tetrahydrofuran cation by VUV-MATI spectroscopy. S. Park, H. Kim, **C. Kwon**

614. Study of absorption intensities in the near infrared region for the first and second overtones of OH and NH stretching vibration with hydrogen bonding. **M. Tatsumi, Y. Morisawa**

615. Study on electrochemical doping in ionic-liquid-gated transistors fabricated with PBT₇T. **I. Enokida***, Y. Furukawa

616. Raman and infrared spectra of a blend of low-bandgap polymer PCPDFTBT and fullerene PC₇₁BM. **M. Kojima, Y. Furukawa**

617. Photoinduced infrared absorption from a blend of PTB7 and PC₇₁BM. **N. Kawate***, Y. Furukawa

618. Electric field effect on the infrared spectra of ferroelectric nylon 11 and 12 films. **H. Isoda***, Y. Furukawa

619. Raman study of tertiary aromatic amines used for organic light-emitting diodes. **Y. Tanaka***, Y. Furukawa

620. Raman investigation of pentacene: Fullerene bulk heterojunction films. **Y. Iwasawa***, Y. Furukawa

621. Analysis of amorphous styrene oligomer using an adiabatic calorimeter as an ultralow frequency spectrometer. **M. Yokota, J. Fujimura, E. Nishiyama, I. Tsukushi***

622. Vibrational analysis for polyenes of various lengths using local mode model and vibrational self-consistent field method. **M. Tsuyuki***, H. Kanamori, S. Yabushita

623. UV resonance Raman studies of membrane protein structure and dynamics. **J. Kim, I. Lopez-Peña, D. Asamoto, G. Kang**

624. Rebinding dynamics of O₂ to heme proteins probed by time-resolved vibrational spectroscopy. S. Park, T. Lee, **M. Lim***

625. Roles of structural changes around Tyr201 in kinase regulation of oxygen sensor protein FixL. **T. YAMAWAKI, H. Ishikawa, M. Mizuno, H. Nakamura, Y. Shiro, Y. Mizutani**

626. Broadband infrared Stokes polarimetry. **W. FitzGerald, D. Hore***

Hawaii Convention Center
313B

Single-molecule Fluorescence Imaging (#208)

Organized by: P. Chen, T. Majima, G. Cosa
Presiding: C. Payne, J. Xiao

19:00 Cell imaging

19:00 – 627. Transcription factor and stochastic gene expression -- perspectives from single molecule studies in live cells. **J. Xiao*, Z. Hensel, X. Fang**

19:25 – 628. Imaging the cellular internalization and transport of nanoparticles. **C. Payne**

19:50 – 629. Investigating membrane protein interactions by single-protein tracking in a single living cell. **N. Lee***

20:15 – 630. Single molecule super-resolution imaging of microtubule bundling in cells expressing rabies virus proteins. **T.D. Bell***, D. Whelan, A. Brice, G.W. Moseley

Hawaii Convention Center
301A

Fundamental Science of Photon and Electron Induced Surface Processes (#228)

Organized by: H. Petek, J. Zhao, Y. Matsumoto
Presiding: A. Migani

19:00 – 631. Time-resolved spectroscopy by optical pump-probe STM. **H. Shigekawa***

19:40 – 632. Theoretical description of photoinduced nonadiabatic dynamics. **Z. Lan***

20:20 – 633. Real-time large scale TDDFT simulations on interface electron-ion dynamics. **S. Meng***

Hawaii Convention Center
312

Interplay between Theory and Experiment in Catalytic Research (#277)

Organized by: M. Ehara, C. Cramer, S. Dai, C. Jones, T. Ziegler, T. Tsukuda

19:00 – 634. A Tribute to Tom Ziegler (1945–2015). **T. Woo***

19:20 – 635. Roles of computational chemistry in understanding base metal organofluorine chemistry. **R. Baker**

19:45 – 636. Understanding catalysis by ligand-protected nanoclusters. **D. Jiang***

20:10 – 637. Search for stable structures in bi-metallic nanoclusters: Application to carbon-halogen bond activation by small gold-palladium clusters. **E. Pahl, M. Ebara, B. Boefka**

20:30 – 638. Electronic structure and catalytic activity of alloy nanoclusters. **R. Fukuda***

20:45 – 639. Chemical machine reasoning for the discovery of new reactions. **M.P. Waller**

Hawaii Convention Center
Halls I, II, III

Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344)

Organized by: D. Kilin, S. Kilina, I. Burghardt, G. Scholes, U. Diebold, A. Selloni, X. Gong, Q. Sun, R. Asahi, K. Dommen

Poster Session
19:00 – 21:00

Dynamics of charge transfer

640. Electron-hole recombination in Sr-doped NaTaO₃ photocatalysts: Solid-state synthesis vs. solvothermal synthesis. **L. An*, H. Onishi***

641. Non-equilibrium charge dynamics in functionalized semiconductor nanostructures. **T. Inerbæv, D. Kilin**

642. Non-radiative relaxation dynamics of photo-induced excitons in (5,0) carbon nanotube and semiconducting PbSe nanowire interface. **A.R. Erck*, W.K. Sapp, D. Kilin**

Properties of doped TiO₂ and perovskites

643. Ga-doped SrTiO₃ photocatalysts prepared via solid-state and molten salt method. **Y. Park, H. Onishi***

644. Theoretical studies of structural and electronic properties of doped BaTaO₂N systems. **H. Iriyuchi*, G. Giorgi, K. Yamashita**

645. Effects of octahedral-tilting and anion ordering on band structures in perovskite tantalum oxynitrides CaTaO₂N and MgTaO₂N. **A. Kubo, G. Giorgi, K. Yamashita**

New non-titania materials for photocatalysis

646. Electronic structure of a metal-organic super container molecule by single point DFT. **W.K. Sapp, A.R. Erck, Z. Wang, D. Kilin**

647. Green synthesis of AgI nanoparticle-functionalized graphene aerogels with enhanced catalytic performance and facile recycling. **A. Devulapalli, J. Choi, R. Ma, T. Kim***

648. Synthesis of AgI-graphene analog boron nitrate nanocomposites as highly efficient photocatalyst for water purification. **J. Choi, A. Devulapalli, R. Ma, T. Kim***

Plasmonic particles

649. Visible light-induced charge separation in heterostructured Au/ZnS nanoparticles. **M. Kimura, M. Sakamoto, A. Furube, H. Adachi, T. Sugimoto, K. Watanabe, Y. Matsunoto, T. Teranishi***

650. Electronic states and photocatalytic activities of titanium dioxide with metal (Au, Pd, Pt) nanoparticles studied by far-ultraviolet spectroscopy. **I. Tanabe*, Y. Ozaki**

651. Development of photoelectrochemical glutathione sensor using Au-TiO₂ nanocomposites. **A. Kuragano, A. Devadoss, P. Sudagar, C. Terashima, K. Nakata, T. Kondo, M. Yuasa, A. Fujishima**

DSSC

652. Density functional theory investigation of Ru/organic dye co-sensitized TiO₂ surface for solar cell application. **V. Otani*, K. Sodeyama, L. Han, Y. Tateyama**

Photocatalytic reactions

653. Selective hydrogenation of furfuril over titanium(IV) oxide photocatalyst. **K. Nakanishi, K. Hashimoto, H. Kominami***

654. Photocatalytic complete oxidative decomposition of acetaldehyde over WO₃ mixed with plant ash under visible light irradiation. **Y. Yamaguchi*, K. Nakata, C. Terashima, K. Sakai, H. Sakai, A. Fujishima**

655. Inactivation mechanism of *Escherichia coli* and Qβ phage with visible-light responsive Rh-doped SrTiO₃ photocatalyst. **S. Usuki, Y. Yamaguchi, K. Nakata, C. Terashima, A. Kudo, T. Suzuki, Y. YOSHIMI, M. Ikekita, A. Fujishima**

656. Photocatalytic hydrogenation of alkenes over organically-modified TiO₂ under visible light irradiation. **S. Kitagawa, Y. Okubo, K. Immura, K. Hashimoto, H. Kominami***

657. Photocatalytic decomposition of common sugar and generation of rare sugars. **Y. Yamamoto, K. Nakata, Y. YOSHIMI, C. Terashima, M. Abe, K. Sakaguchi, M. Ikekita, A. Fujishima**

658. Photo-electrochemical reduction of CO₂ using photocatalyst anode-boron doped diamond cathode hybrid system. **N. Chikamori*, K. Nakata, C. Terashima, Y. Einaga, A. Kudo, H. Sakai, K. Sakai, A. Fujishima**

Applications and devices

659. Field and laboratory performance tests of an air-cleaner with photocatalysis-plasma synergistic reactors for practical and long-term use. **T. Ochiai*, N. Nishida, T. Machida, Y. Uchida, A. Fujishima**

660. Development of purification technology in the plant factory using visible-light driven photocatalysts. **T. Sanada*, C. Terashima, K. Nakata, T. Kondo, M. Yuasa, A. Fujishima**

661. Ammonia synthesis by liquid plasma processing under nitrogen stream. **K. Honda*, C. Terashima, K. Nakata, T. Kondo, M. Yuasa, A. Fujishima**

662. Design of photocatalysts for efficient inactivation of *E. coli*. **T. Shimoda, M. Ikekita, K. Nakata, C. Terashima, Y. YOSHIMI, A. Fujishima, S. Usuki**

663. Inactivation of *Microcystis aeruginosa* by TiO₂ photocatalysis. **K. Kanagawa*, K. Nakata, Y. YOSHIMI, C. Terashima, M. Ikekita, A. Fujishima**

Hawaii Convention Center
Halls I, II, III

Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370)

Organized by: W. Zhao, W. Zhuang,

M. Cho, G. Sholes

Presiding: M. Cho, G. Scholes, W. Zhao, W. Zhuang

Poster Session

19:00 – 21:00

664. Using 2DIR spectroscopy for label free analysis of drug protein interactions. **H. Sowley***

665. Phase-modulated coherent spectroscopy applied to ultracold doped helium droplets. **L. Bruder, M. Binz, M. Mudrich, F. Stienkemeier***

666. Femtosecond time-resolved spectroscopy of various IR probes for studying structure and dynamics of myoglobin, reverse micelles, and peptides. **M. Maj, K. Kwak, H. Han, M. Cho***

667. Frequency fluctuations of non-ionic vibrational probe molecule in water studied by 2D infrared spectroscopy and molecular dynamics simulation. **M. Okuda*, M. Higashi, K. Ohta, S. Saito, K. Tominaga**

668. Use of 2D infrared spectroscopy for the quantification and spatial mapping of post-translation modifications of proteins. **L. Rezende Valim*, J.A. Davies, K.R. Willison, D.R. Klug**

669. Determination of second hyperpolarizability with computational Raman activities and identification of DOVE signatures for selected molecules. **W. Zhao***

Hawaii Convention Center
310 Theatre

Frontiers of Plasmon Enhanced Spectroscopy (#428)

Organized by: Y. Ozaki, Z. Tian, B. Ren, N. Halas, A. Brolo, T. Itoh, M. Moskovits

Presiding: Z. Tian

19:00 – 670. Photobleaching of fluorophores in surface-enhanced spectroscopies. **E. Le Ru***

19:20 – 671. Plasmonic scattering of linear nanoantennas and vibrational coupling in the infrared. **C. Huck, J. Vogt, A. Pucci***

19:50 – 672. Mid-IR plasmonics for chemical specific and ultrasensitive biosensing. **H. Altug, D. Etezadi, O. Limaj, D.L. Rodrigo**

20:10 – 673. Plasmonic nanoparticles and metasurfaces for sensing and spectroscopy. **M. Kall**

20:30 – 674. Tip-enhanced Raman spectroscopy: A nanospectroscopy for surface sciences and electrochemistry. **B. Ren*, Z. Zeng, X. Wang, J. Zhong, S. Huang, T. Huang, M. Li**

20:55 Closing Remarks

* Principle Author

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Hawaii Convention Center
307AB

Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)

Organized by: H. Sekiya, T. Zwier,
M. Fujii, E. Bieske, N. Kim
Presiding: H. Sekiya

- 19:00 – 675. Study on hydrogen-bonded structures of acetylene large clusters by 2D correlation IR spectroscopy.
Y. Matsumoto*, R. Yoshiura, K. Honma
19:20 – 676. Stalking higher energy conformers on the potential energy surface of charged species. **M. Gaigeot***
19:40 – 677. Spectroscopic studies on host-guest complexes in the gas phase and on gold surface. **Y. Inokuchi***
20:00 – 678. Resonance enhanced photo-dissociation spectra of the $\text{H}_2\text{C}_2\text{H}^+$ -Ne and $\text{H}_2\text{C}_2\text{H}^+$ - N_2 complexes. K. Catani, J. Sanelli, V. Dryza, P. Taylor, **E. Bieske***
20:25 – 679. Watching solvent migration dynamics in clusters by picosecond time-resolved IR spectroscopy. **M. Fujii***

Hawaii Convention Center
306A

Interplay between Chemistry and Dynamics in Biomolecular Machines (#441)

Organized by: S. Hayashi, A. Kitao,
Y. Rhee, E. Tajkhorshid
Presiding: S. Hayashi

- 19:00 – 680. Structures and functions of macromolecular motor assemblies.
K. Namba*
19:30 – 681. Entropy-driven biological processes: Signaling mechanisms in controlled entry of viruses into host cells.
S. Varma*, M. Bottani, N. Duro, P. Dutta, R. Leighty
19:50 – 682. Xenobiotic recognition and efflux control by bacterial cells.
M. Hayashi-Nishino, K. Hayashi,
T. Fujioka, Y. Takeuchi, S. Yamasaki,
A. Yan, **K. Nishino**
20:10 – 683. Structure, dynamics, and function of bacterial flagella investigated by molecular dynamics simulation. **A. Kitao***
20:40 Closing Remarks

Thursday Morning

Hawaii Convention Center
Halls I, II, III

Synergistic Relationships between Computational Chemistry and Experiment (#9)

- Organized by: S. Wetmore, H. III,
L. Radom, P. Schwertfeger, R. Wah,
H. Nakai, K. Kim
Poster Session
10:00 – 12:00
684. Rotational spectrum and quantum chemical calculations for methyl trimethyl acetate. **Y. Tajimi**, R. Nomura, N. Kuze
685. Theoretical study on cobalt-catalyzed transformation of molecular dinitrogen into silylamine. **H. Tanaka***, R. Imayoshi,
Y. Matsuo, M. Yuki, K. Nakajima,
K. Yoshizawa, Y. Nishibayashi
686. Active site genesis within UIO-66 type metal-organic frameworks: A theoretical rationalization. **M. Vandichel**, J. Hajek,
A. Ghysels, M. Waroquier, D. De Vos,
V. Van Speybroeck
687. Computational-aided understanding and design of 2D graphene-like materials. **J. Wang**
688. Intramolecular C–H activation reactions of Ru(NHC) complexes combined with H₂ transfer to alkenes: A theoretical elucidation of mechanisms and effects of ligands on reactivities. **K. Wenz**, P. Liu,
K.N. Houk*
689. Structure of (H₂O)_{2n}: Quantum chemical exploration of stable structures.
M. Takagi, S. Maeda, T. Taketsugu

690. Examining structure-function relationships in DNA repair facilitated by adenine DNA glycosylase. **S. Lenz**, S. Wetmore*
691. Effects of adduct linkage on DNA replication: A computational investigation of the benzyl-guanine and pyridylloxobutyl-guanine adducts. **K. Wilson**, S. Wetmore*
692. Molecular dynamics study of the hogg1 and Fpg DNA repair enzymes.
S. Sowlati-Hashjin, S. Wetmore*
693. Cobalt and zinc complexes of hexaamine cage ligands with multiple conformations in solution. **L.J. Alcock**,
G. Cavigliasso, R. Stranger, A.C. Willis,
J. Hook, D. Lawes, S.F. Ralph
694. Theoretical study on photoabsorption properties of unsubstituted boron-dipyromethene (BODIPY). **M. Asaoka**,
K. Miyagi, T. Takebayashi, Y. Kitagawa,
M. NAKANO
695. Accurate calculation of standard enthalpies of formation of carboxylic acids and derivatives. **R. Bacaloglu***
696. Computational study of *trans*-(E)-4-(2-(pyridin-2-ylvinylbenzoic acid and *trans*-(E)-4-(4-(pyridin-4-ylvinylbenzoic acid. **M. Castro***, M.J. Percino,
J. Soriano, M. Ceron, V. Chapel
697. Probing thermomolecular orientation and fluid polarization by terahertz spectroscopy: Molecular dynamics simulations and experiments. **C.D. Daub***,
R. Zamiri, U.L. Österberg, P. Åstrand,
F. Bresme
698. Analysis of Al organization in zeolites by multinuclear MAS NMR and QCH calculations. **D. Dedecek**, S. Sklenak, P. Klein
699. Combining experimental and computational techniques to investigate complex mineral structures: The multiple structures of vaterite. **R. Demicheli***,
M. De La Pierre, R. Raiteri, J.D. Gale,
U. Wehrmeister, D.E. Jacob
700. Computational modeling of PHR functional conversion. **H. Dokainish**,
D. Yamada, t. iwata, H. Kandori, A. Kitao*
701. Development of experiment and theory to detect and predict ligand phase separation on silver nanoparticles. **S. Egorov***,
D. Green, Z. Farrell, S. Merz
702. Structure and vibrational spectra of solid-liquid and liquid-air interfaces, including electrolytes, with DFT-based molecular dynamics simulations. **M. Gaigeot***
703. Anharmonic vibrational spectroscopy of gas phase molecules and clusters: Synergy between DFT-MD simulations and IR-MPD/IR-PD experiments. **M. Gaigeot**
704. Theoretical study on the cavity effect of semihollow-ligands in gold(I)-catalyzed alkyne cyclizations. **M. Gao***, S. Maeda,
T. Iwai, M. Sawamura, T. Taketsugu
705. Intrinsic electrophilicity of oxalic acid monomer is enhanced in the dimer and trimer by intermolecular proton transfer. **M. Gutowski**, Z.G. Keolopile,
M.R. Ryder, M. Haranczyk,
A. Buonaugurio, J. Graham,
A. Bulyendy, K.H. Bowen
706. Proton delocalization and structure-specific fluorescence in amyloid fibrils. **A. Hassanal***, D. Pinotsi, L. Grisanti,
P. Mahou, R. Gebauer, C. Kaminski,
G. Kaminski
707. Experimental and computational investigation of the transition states for the 1,1-HCl and 1,1-HF elimination reactions from chemically activated CD₃CHFCI molecules. **B.E. Holmes***, G. Heard,
T. Brown, M. Nestler
708. DFT study of the hydrogenation of N₂ with H₂ to NH₃ by heterolytic outer sphere cleavage of H₂ between tungsten dinitrogen complexes and cationic rhodium dimers: Is a molecular Haber-Bosch catalyst in sight?. **M. Hölscher***,
V. Moha, W. Leitner
709. Desk-top tool for eco-toxicity prediction of chemical substances. **Y. Inagaki***,
T. Yamazaki, Y. Takahashi
710. Artificial intelligence tool for classification of chemical structures. **A. Iwamoto***,
Y. Takahashi
711. Vibrational properties and energy redistributions in hydrogen bonded clusters obtained from ab initio dynamics simulations. **S.S. Iyengar**
712. Molecular dynamics of designed and evolved enzymes. **G. Jimenez-Oses**,
S. Osuna, K.N. Houk
713. Theoretical study on electron conductivities of 1D nickel(II) complexes.
Y. Kitagawa, T. Takebayashi, M. Asaoka,
K. Miyagi, Y. Shigeta, M. NAKANO
714. Effects of the anharmonic vibrational corrections on molecular structures of acetates and oximes: Gas-phase electron diffraction and quantum-chemical studies. **N. Kuze***, Y. Tajimi, A. Ishikawa
715. Infrared multiphoton dissociation spectroscopy and density functional theory (DFT) studies of protonated permethylated β -cyclodextrin-water non-covalent complexes. **S. Lee**, H. Oh, S. Lee
716. Molecular dynamics simulations with polarizable and reactive force fields for treating conformation changes and reactions in condensed phase. **J. Ma***
717. Solution-phase dynamics of Thioflavine T: Experiment and computation.
J. Breffke, B. Conway, **M. Maroncelli***
718. Single-molecule piezoelectrics: A novel approach to energy harvesting materials. **C.W. Marvin***, G. Hutchison
719. Electrostatic effects of the magnesium ions on the catalysis of critical mutants of the DNA Polymerase β . **R.A. Matute***,
A. Warshel*
720. Rational design of inhibitors targeting human β -galactoside α -2,6-sialyltransferase I. **A. Montgomery**, R. Szabo,
H. Yu, D. Skropeta
721. Electronic structure properties of nano-hybrid supercapacitive materials comprising polyoxometalate Keggin-like structures deposited on graphene: A DFT study. **J. Muniz***, A.K. Cuentas-Gallegos,
M. Robles, M. Valdez
722. Theoretical study of isomerization process of fluvoxamine. **k. ODAI***, E. Ito
723. Study on ultrafast excited states dynamics of ortho-nitroaniline using femtosecond transient absorption spectroscopy. **T. Yi*, X. Pu***, M. Li*
724. Facile C_{sp2}-C_{sp2} bond cleavage in oxalic acid-derived radicals. R. Molt,
T. Clark, R. Bartlett, **N. Richards***
725. ⁷Li-NMR for corannulene sandwich-like aggregates: One molecule, three signals, two records. **A. Rogachev***
726. Structural and electronic properties of pristine and doped polythiophene: Periodic vs. molecular calculations. **T.P. Kaloni**, **G. Schreckenbach***,
M.S. Freund
727. Lead discovery of telomerase inhibitors using virtual screening technique. **D. Song***, J. Yang, G. han
728. Pressure-induced deformations of the energy surfaces of compressed species and reaction systems. **J.A. Spooner***,
N. Weinberg*
729. Electronic-structure-based chemoinformatics for molecular design and discovery. **M. Sugimoto***
730. Kinetic analysis for complex reaction networks: Application to organic reactions. **Y. Sumiya***, S. Maeda,
T. Taketsugu
731. Quantum-chemical calculations of the scalar-pseudoscalar interaction in heteronuclear diatomic molecules. **A. Sunaga**,
M. Abe*, B. Das, M. Hada

- Hawaii Convention Center
308A
- Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44)**
- Organized by: S. Tretiak, G. Chen,
Y. Tanimura
Presiding: S. Tretiak
- 8:00 Opening Remarks
8:05 – 732. Theoretical exploration of excitation energy transfer and charge separation dynamics in photosystem II.
D.F. Coker*, P. Huo, J. Moix, J. Cao
8:35 – 733. Quantum coherence in transport processes. **J. Cao***
9:05 – 734. Excited state nonadiabatic molecular dynamics in chlorophylls.
S. Fernandez Alberti*,
L. Alfonso-Hernandez, P. Shenai,
Y. Zhao, S. Tretiak
9:35 – 735. Benchmarking calculations of excitonic couplings between chlorophylls. E. Kenny, **I. Kassal**
9:55 Break
10:10 – 736. Optical dynamics and coherence of excitons in natural and synthetic molecular aggregates. **J. Kroester***
10:40 – 737. Characterization of excited state properties of molecular substituents using geometry and topology. **V.Y. Chernyak***
11:10 – 738. Vibronic spectra of organic aggregates and molecule-metallic nanoparticles. **W. Liang***
11:40 – 739. Ammonia and cesium adsorption on Keggin-type molybdocephosphate studied by density function quantum chemistry calculations and batch experiments. **Z. Tan***, D. Lan*, Z. Huang*,
X. Wang*
- Hawaii Convention Center
Halls I, II, III
- Multiscale Couplings of Molecular Theory of Solvation: Fundamentals and Applications (#60)**
- Organized by: A. Kovalenko, B. Pettitt,
F. Hirata
Presiding: F. Hirata, A. Kovalenko,
M. Pettitt
- Poster Session**
10:00 – 12:00
740. Free energy calculation for the ATP-induced dimerization of the nucleotide-binding domains in a maltose transporter: Importance of the water-mediated entropic force. **T. Hayashi**, S. Chiba,
T. Furuta, **M. Sakurai***
741. Theoretical prediction of mutations leading to enhanced structural stability of GPCRs. **Y. KAJIWARA**, S. Yasuda,
Y. TAKAMUKU, N. SUZUKI, T. MURATA,
M. Kinoshita
742. Effects of cosolvent addition on the thermal stability of a protein. **S. Murakami***, M. Kinoshita
743. 3D-RISM study of water-mediated forces between the nucleotide binding domains responsible for the power stroke in an ABC transporter.
T. Furukawa-Hagiya, N. Yoshida,
S. Chiba, T. Hayashi, T. Furuta,
M. Sakurai*
- Hawaii Convention Center
Halls I, II, III
- Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)**
- Organized by: J. Hasegawa, M. Collins,
M. Gordon, P. Piecuch, T. Taketsugu
Presiding: J. Hasegawa
- Poster Session**
10:00 – 12:00
744. Quantum chemical calculations for the excited states of *para*-methylcinnamate (p-MMC). **J. Kim***, J. Moon

* Principle Author

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- 745.** Broad range electronic spectra of large molecules by simplified TD-DFT and TDA-DFT. **S. Grimme***
- 746.** Excited state calculations with exact-exchange Kohn-Sham orbitals. **K. Hong**, J. Kim, S. Choi, S. Hwang, W. Kim*
- 747.** Computed structures and energetics of *para*-propylaniline complexes with one and two argon atoms: A basis for interpretation of electronic and cationic spectra. **C. Trindle***, Q. Gu, J. Knee
- 748.** Constricted variational density functional theory (CV-DFT): Idea and recent applications. **F. Senn***, Y. Park, M. Krykunov, I. Seidu, T. Ziegler
- 749.** Optimization of complex orbital exponents by analytical gradient method for photoionization differential cross sections. **R. Matsuzaki**, S. Yabushita
- 750.** Epoxidation reactions of alkenes using iron(IV)-oxo porphyrin π -cation species: A SO-CASPT2 study. **K. Ujaki**, M. Abe, H. Fujii, M. Hada
- 751.** Introducing a numerical stable Δ SCF-DFT scheme based on the constricted variational density functional theory: Triplet calculations. **Y. Park**, F. Senn, M. Krykunov, T. Ziegler*
- 752.** All-electron first-principles X-ray adsorption spectra calculations for acetone and acetic acid. **Y. Noguchi***, M. Hiyama, H. Akiyama, Y. Harada, N. Koga
- 753.** Excited-state dynamics of *trans*-aminostibile derivatives. **H. Yao***, L. Cheng, J. Yang, I. Chen
- 754.** Beyond semiclassics for heavy particle dynamics in chemical reactions. **S. Takahashi***, K. Takatsuka
- 755.** Recent progress in ab initio multiconfigurational Ehrenfest method for molecular dynamics study. **K. Saita**, A. Kirrander, D.V. Shalashilin
- 756.** Theoretical and experimental investigations on near-infrared absorption of trioxatriguadine derivatives with pi-stacked columnar structures. **Q. Wang**, Y. Ikabata, T. Yoshikawa, A. Ueda, T. Murata, K. Kariyazono, H. Okamoto, Y. Morita, H. Nakai
- 757.** Combined molecular beam and matrix isolation methodology for the separation, trapping, and storage of nuclear spin isomers of water. **J. Vermette**, P. Turgeon*, P. Ayotte, G. Alexandrowicz
- Hawaii Convention Center
304A
- Self-organization in Chemistry (#165)**
- Organized by:* S. Nakata, J. Pojman, O. Steinbock, Q. Gao, J. Wang, T. Yamaguchi, R. Yoshida, S. Nakabayashi
Presiding: S. Nakata, O. Steinbock, J. Wang
- 8:00** Opening Remarks
- 8:05 – 758.** Pattern formation in structured media. **I.R. Epstein**
- 8:35 – 759.** Metabolic network and glycolytic oscillations in yeast and cancer cells. **T. Amemiya***, K. Obase, N. Hiramatsu, K. Itoh, K. Shibata, M. Takinoue, T. Yamamoto, T. Yamaguchi
- 8:55 – 760.** Interaction between bromate-based chemical oscillators and noble metal nanoparticles. **J. Wang**
- 9:15 – 761.** Spectrophotometric study of the Belousov-Zhabotinsky batch pH oscillator. **G. Frerichs***, Y. Chen
- 9:30 – 762.** Liesegang patterns produced by reduction reaction of metal ions. **H. Nabika***, M. Sato, Y. Shimizu, K. Unoura
- 9:45 coffee break**
- 10:00 – 763.** Morphology and phase separation kinetics of polymer mixtures driven by photopolymerization: Summary and perspectives. **Q. Tran-Cong-Miyata**
- 10:30 – 764.** Synchronization and travelling waves of sulfur electro-deposition in the regions of passivation and transpassivation. **Q. Gao***, J. Yang, W. Bi, Y. He
- 10:50 – 765.** Planetary atmospheres as self-organising systems based on Clausius' virial theorem. **I.R. Kennedy***

- 11:10 – 766.** Perturbing Turing patterns formed by the chlorine dioxide-iodine-malonic acid reaction with halide salts. **D. Gaskins**, E. Pruc, M. Dolnik, I.R. Epstein*
- 11:25 – 767.** Variation in dynamics of BZ reaction under various sets of chemical composition in catalyst and organic substrates. **Y. Mori**, F. Faqiryar, T. Fukuda, T. Matsumura*
- 11:40 – 768.** Self-motion of aspirin crystals at the air-water interface. **A.F. Taylor***, T. Bansagi
- 11:55 Discussion**
- Hawaii Convention Center
310 Theatre
- Recent Progress in Matrix Isolated Species (#199)**
- Organized by:* T. Momose, Y. Lee, D. Anderson
Presiding: D.T. Anderson, S.A. Reid
- 8:00 – 769.** Solvation of atomic dopants in solid parahydrogen: Quantum Monte Carlo studies. **R. Hinde***
- 8:30 – 770.** High-resolution IR laser kinetic spectroscopy of $\text{CH}_2\text{F}-\text{ortho-H}_2\text{O}$ cluster in solid *para*- H_2 . **H. Kanamori***
- 9:00 – 771.** Helium droplet assisted preparation and spectroscopy of alkali-alkaline earth diatomics. F. Lackner, J.V. Pototschnig, **W.E. Ernst***
- 9:15 – 772.** Insights from the application of the full-configuration-interaction nuclear-orbital approach to small doped ^3He , ^4He and *para*- H_2 clusters. **M. De Lara-Castells***, A. Mitrushchenkov
- 9:30 – 773.** Molecular dynamics in parahydrogen matrices. **C. Crepin***
- 10:00 Break**
- 10:15 – 774.** Spectroscopy of isolated molecules and chemistry in space-time. **V.A. Apkarian***
- 10:45 – 775.** Spatial manipulation of amplitude and phase distribution of vibrational excitations in solid para-hydrogen. **H. Katsuki***
- 11:15 – 776.** Multiscale simulations of dynamic processes in argon matrices. **E. Sanchez-Garcia***, M. Fernandez-Oliva, K. Bravo-Rodriguez, W. Sander
- 11:30 – 777.** Superradiance of organic molecules attached to rare gas clusters. **F. Stienkemeier***, M. Müller, S. Izadnia, A. LaForge, A. Eisfeld
- 11:45 – 778.** Coherent frequency conversion using quantum solid. **Y. Miyamoto**
- Hawaii Convention Center
306B
- Metal Ions and Protein Functions: Theoretical Models and Applications (#202)**
- Organized by:* Q. Cui, M. Meuwly, T. Allen, Y. Gao
Presiding: Q. Cui
- 8:00 – 779.** Selective recognition of heavy elements by protein-based reagents. **C. He***
- 8:40 – 780.** Principles governing biological processes: Applications to drug design and drug target identification. **C. Lim***
- 9:20 – 781.** Zn coordination chemistry: Validation of the XYG3 type of doubly hybrid density functionals. N. Su, **X. Xu***
- 10:00 Break**
- 10:15 – 782.** Polarizable molecular mechanics and quantum chemistry analyses of polyligated complexes of mono- and polyvalent metal cations: Alkali, alkaline-earth, transition, and heavy metal cations. **N. Gresh***
- 10:55 – 783.** Accelerating metal-directed protein folding and molecular recognition with enhanced sampling techniques. **F. Feixas***, M. Swart
- Hawaii Convention Center
312
- Interplay between Theory and Experiment in Catalytic Research (#277)**
- Organized by:* M. Ehara, C. Cramer, S. Dai, C. Jones, T. Ziegler, T. Tsukuda
- 8:00 – 800.** Recent material development for photocatalysis. **S. Dai***, J. Zhang
- Hawaii Convention Center
313B
- 8:20 – 801.** Combining theory and experimental validation in the use of TEMPO for anodic electrocatalysis. **S. Minteer***, D. Hickey, M. Sigman, D. Schiedler, M. McCammant, I. Matanovic, P. Atanassov
- 8:45 – 802.** CO_2 fixation mechanism of bi-functional porphyrin catalyst: A theoretical study. **J. Hasegawa**
- 9:10 – 803.** Bioinspired computational design of iron pincer complexes for base free hydrogenation of carbon dioxide. **X. Yang***
- 9:25 – 804.** Unraveling the enantioselectivity-controlling surface processes in the proline-mediated isophorone hydrogenation on Pd supported catalyst. **L. Rodriguez Garcia***, F. Meemken, K. Hungerbühler, A. Balter
- 9:40 Break**
- 9:55 – 805.** Combined theoretical and experimental studies on cyclohexene oxidation reaction: C–H activation reactions are not as simple as you thought. **K. Cho***, Y. Kim, S. Shaik, W. Nam
- 10:20 – 806.** Highly efficient photo-SCR of NO with ammonia. **T. Tanaka***, A. Yamamoto, T. Shishido, K. Teramura
- 10:45 – 807.** Design and applications of single-site photocatalysts using nanoporous materials. **H. Yamashita***
- 11:10 – 808.** Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells. **S. Linic**
- 11:35 – 809.** Unique reactivity and in-situ synthesis of oxide-supported single atom Rh catalysts. **P. Christopher***
- Hawaii Convention Center
306A
- Science with Beams of Radioactive Isotopes (#340)**
- Organized by:* S. Yennello, K. Starosta, Y. Zhao, H. Haba
Presiding: K. Starosta
- 8:00 Welcome**
- 8:05 – 810.** Nuclear science: Exploring the heart of matter, serving society, and educating the next generation of innovators. **A. Abrahamian***
- 8:35 – 811.** Scientific programs with exotic nuclei at RIBF. **H. Sakurai**
- 9:05 – 812.** Nuclear science program at ISAC/TRIUMF. **J. Dilling***
- 9:35 – 813.** Transitioning NSCL into FRIB at MSU. **C. Gelbke***
- 10:00 break**
- 10:15 – 814.** Radioactive beam facilities in Europe - current status and future perspectives. **P. Egelhof***
- 10:40 – 815.** Nuclear astrophysics experiment at China Jinping underground Laboratory. **X. Tang**
- 11:05 – 816.** Nuclear forces and their impact on matter at neutron-rich extremes. **A. Schwenk**
- 11:30 – 817.** Use of radioactive beams for the synthesis of the heaviest elements. **W. Loveland***
- 12:00 Lei Yang**

* Principle Author

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Hawaii Convention Center
305B

Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344)

Organized by: D. Kilin, S. Kilina,
I. Burghardt, G. Scholes, U. Diebold,
A. Selloni, X. Gong, Q. Sun, R. Asahi,
K. Domnen
Presiding: D. Kilin, B.A. Parkinson

- 8:00** Introductory Remarks: Photocatalysis Symposium #344
8:05 – 818. Water splitting by thin film metal-oxo catalysts. **D.G. Nocera**
8:35 – 819. Theoretical study of N-doped Ta_2O_5 /Ru-complex system for photocatalytic CO_2 reduction. **R. Asahi***,
A. Akimov, R. Jinnochi, S. Shirai,
O. Prezhdo
9:05 – 820. First principles simulations of materials and processes in photocatalysis. **A. Selloni**
9:35 – 821. NO adsorption and diffusion on hydroxylated rutile $TiO_2(110)$: electron trapping and transferring. **Y. Yu, X. Gong***
10:00 – 822. Cobalt doped TiO_2 : A computational analysis of surface dopant placement on anatase. **S. Jensen***, D. Kilin
10:15 Break
10:30 – 823. Efficient water splitting on photoelectrodes with surface modifications. **K. Domnen***
11:00 – 824. Predicting photocatalytic materials: Condensed matter physics meets electrochemistry. **G. Galli***
11:30 – 825. Suspended inorganic nanostructures for photocatalytic water splitting. **F. Osterloh**

Hawaii Convention Center
301B

Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370)

Organized by: W. Zhao, W. Zhuang,
M. Cho, G. Sholes
Presiding: W. Zhuang

8:00 – 826. Detection modes of vibrational and electronic coherence in multidimensional stimulated Raman signals. **S. Mukamel***, K. Bennett, H. Ando,
B. Agarwalla, K. Dorfman
8:25 – 827. Multidimensional coherent optical photocurrent spectroscopy of a semiconductor microcavity. **S. Cundiff***
8:50 – 828. Structure and dynamics at electrode/catalyst interfaces probed by time-resolved vibration sum-frequency generation spectroscopy. **T. Lian**
9:15 – 829. Femtosecond stimulated Raman spectroscopy by six-wave mixing. **A. Moran**
9:40 – 830. Fifth order coherent multidimensional optical spectroscopies. **H. Tan***
10:05 Break
10:20 – 831. Fourier transform multidimensional vibrational-electronic spectroscopies. **T.L. Courtney, Z. Fox, J.D. Gaynor, M. Balasubramanian, M. Khalil**
10:45 – 832. Surface-specific 2D vibrational spectroscopy reveals dynamics of interfacial water. **M. Bonn***
11:10 – 833. 2D white-light spectroscopy reveals exciton dynamics in next-generation solar cells. **T.J. McDonough*, R.D. Mehlenbacher, N.M. Kearns, M. Wu, M. Grechko, M.S. Arnold, M.T. Zanni**
11:35 – 834. Probing structure and dynamics of preferential solvation in biomolecular hydration and photocatalysis using ultrafast 2D-IR spectroscopy. **K. Kubarych**

Hawaii Convention Center
305A

Practical Strategies for Modeling Non-Covalent Interactions (#372)

Organized by: G. Beran, Y. Jung,
H. Nakai, J. Schmidt
Presiding: Y. Jung

8:00 Introduction

- 8:10 – 835.** Modeling noncovalent interactions with RPA-type methods. **V.K. Voora, G.P. Chen, M.M. Agee, B.S. Ganesh, F. Furche***
8:40 – 836. Energetics of nanolayer structures from semi-analytic RPA-level theory. **J. Dobson***, T. Gould, S. Lebegue
9:10 – 837. Cost effective quantum chemical methods for organic crystal modeling. **G. Brandenburg**, S. Grimmel
9:30 – 838. Properties of racemic and enantiopure crystals from density-functional theory. **E.R. Johnson***, A. Otero-de-la-Roza, J. Hein
10:00 Break
10:10 – 839. Toward large-scale quantum chemical calculations with static and dynamical electron correlations. **M. Kobayashi***, T. Taketsugu
10:40 – 840. Density-dependent dispersion correction for density functional theory: Local response dispersion approach. **Y. Ikabata***
11:10 – 841. Performance of BLYP can be significantly improved when used with both dispersion-correcting potentials and pair-wise dispersion corrections. **G. DiLabio***, J. van Santen
11:30 – 842. Improving accuracy and feasibility for density functional calculations in molecules and solids. **Y. Jung**
- Hawaii Convention Center
304B
- Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403)**
- Organized by:* A. Amirfazli, Y. Zuo, J. Li
Presiding: A. Amirfazli, R. David, F. Duan, L. Jiang
- 8:00** Welcome
8:05 – 843. Splashing criterion for impact of complex drops. V. Grishaev, C.S. Iorio, **A. Amirfazli***
8:35 – 844. Branch-shaped particle assembly in drying a sessile colloidal droplet. A. Crivoli, X. Zhong, **F. Duan***
9:00 – 845. Droplet dynamics under the effect of airflow on superhydrophobic surfaces. **A. Dolatabadi***
9:20 – 846. Effect of contact angle on the orientation, stability, and assembly of dense floating cube. M. Donnell, R. Daniello, **J.P. Rothstein**
9:40 Coffee Break
9:50 – 847. Bioinspired interfacial materials with super-wettability. **L. Jiang***, W. Guo, L. Wen, Y. Tian
10:15 – 848. Theoretical model for interfacial tensions between low-energy liquids and solids. **R. David***, A. Neumann
10:40 – 849. Reversible switching between contrasting Cassie and Wenzel states. **A. Luzar**, D. Vanzo, D. Bratko
11:00 – 850. Dynamics of spreading on microtextured surfaces. **A. Mohammad Karim**, H. Kavehpour
11:20 – 851. Effect of surface energy on ice-phobicity. **E. Alizadeh-Birjandi**, H. Kavehpour
- Hawaii Convention Center
Halls I, II, III
- Frontiers of Plasmon Enhanced Spectroscopy (#428)**
- Organized by:* Y. Ozaki, Z. Tian, B. Ren, N. Halas, A. Brolo, T. Itoh, M. Moskovits
Presiding: M. Fujii, H. Sekiya
- Poster Session**
10:00 – 12:00
- 852.** Polyethylenimine-capped gold nanoparticle film with controlled interparticle distance: Preparation, characterization, and application as SERS substrate. **K. Shin***
853. Study of molecular behavior in dark SERS state by using power law analysis of blinking SERS. **Y. Kitahama***, D. Araki, Y.S. Yamamoto, T. Itoh, Y. Ozaki
854. Semiconductor-enhanced Raman scattering for monitoring the small inorganic molecule and ion. **W. Ji***, Y. Wang*, . Tanabe*, **B. Zhao***, Y. Ozaki
- 855.** Plasmon-induced ultrafast electronic dynamics in dye molecules showing surface-enhanced fluorescence. **T. Itoh***, Y.S. Yamamoto, H. Tamaru, V. Biju, S. Wakida, Y. Ozaki
856. Surface-enhanced hyper-Raman scattering for accessing two-photon molecular properties. **H.K. Turley***, J. Camden
857. Exploring Fano interferences of mixed metal nanoparticles. **S. Griffin**
858. Gold nanoparticle self-assemblies for on-dose-authentication of medical tablets. **T. Fukuoka**, A. Yamaguchi, Y. Utsumi, Y. Mori
859. Highly sensitive SERS detection for CBR materials. Y. Park, S. Jin, H. Hwang, J. Lee, **Y. Jung***
860. Biocompatible SERS nanoprobe for immunosorbent assay. L. Chen, Y. Sa, Y. Park, X. Wang, B. Zhao, **Y. Jung**
861. Chlorophenol molecularly imprinted polymer synthesis and application on SERS detection. **Y. Xie***
862. Development of concavo-convex graphene aimed at controlling phonon mobility and their property evaluation by TERS. **Y. Wada***, S. Uemura, Y. Ozaki, S. Vantasin, B. Jayedavan, T. Itoh, Y. Sunayama
863. Exploring intranuclear molecular information by SERS spectroscopy. **L. Liang, S. Xu, W. Xu***
864. Fabrication of SERS substrates based on a hierarchical structural AAO template. **Y. Wang, W. Xu, S. Xu***
865. Online combination of high performance liquid chromatography with surface-enhanced Raman spectroscopy. W. Wang, M. Xu, **Y. Yuan***, J. Yao*
866. Improving the SERS detection on aromatic molecules by PDMS coated Au nanoparticle monolayer film. C. Qian, **Y. Yuan***, Q. Guo, J. Yao*
867. 3D SERS imaging using chemically synthesized nanoporous silver microparticles with highly symmetric geometry. **S. Vantasin**, H. Gatemala, Y. Tanaka, W. Ji, K. Wongravee, S. Ekgasit*, Y. Ozaki*
868. Rational fabrication of AFM TERS tips by electrodeposition method. **T. Huang***, L. Yang, Z. Zeng, M. Li, X. Wang, F. Yang, B. Ren
869. Surface-enhanced Raman scattering from size-controlled PbS quantum dots at gap of Au nanodimer. **X. Li***, K. Suzuki, T. Yoshii, S. Yasuda, K. Murakoshi
870. Tip-enhanced Raman spectroscopy of monolayer graphene island grown on 4H-SiC (0001) C-face. **S. UEMURA**, Y. Tanaka, Y. Kutuma, S. Vantasin, T. Kaneko, Y. Ozaki
871. Facile synthesis and characterization of silver nanoparticles produced by short-chain triazine derivatives and cationic surfactant. **J. Kurawaki**, R. Usman, Y. Niidome
872. Sterically-bulky self assemblies of gold nanoparticles. **T. Fukuoka***, R. Takahashi, Y. Utsumi, A. Yamaguchi
- Hawaii Convention Center
Halls I, II, III
- Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)**
- Organized by:* H. Sekiya, T. Zwier, M. Fujii, E. Bleske, N. Kim
Presiding: M. Fujii, H. Sekiya
- Poster Session**
10:00 – 12:00
- 873.** Relaxation dynamics following the photoexcitation of the $I(H_2O)_4$ cluster. **W. Sheu***, M. Chiou
874. IR spectroscopy of 5-hydroxyindole-methanol in the gas phase: Rearrangement of H-bond. **K. Yoneyama**, K. Sakota*, H. Sekiya
875. Rearrangement of hydrogen bond network in mono-hydrated 5-hydroxyindole cluster cations. **T. Ikeda***, K. Sakota, H. Sekiya

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891. Machinery of new eubacterial light-driven pumps: Sodium and chloride pump rhodopsins. **K. Inoue**, Y. Kato, A. Mori, R. Abe-Yoshizumi, H. Kandori*

892. Plausible model for the inward-facing conformation of ADP/ATP carrier: A simulation study. **K. Tamura**, S. Hayashi*

893. Structural and functional roles of coupling helices in ABC transporter MsbA: Experimental and computational studies. **T. Furuta**, T. Yamaguchi, H. Kato, M. Sakurai

894. Molecular mechanism of Ca^{2+} -induced membrane fusion: A molecular dynamics study. **H.G. Tsai**

895. Analysis of the free energy landscape for the open-close dynamics of maltose transporter ATPase, MalK, using enhanced sampling MD simulation. **W. Hsu**, T. Furuta, M. Sakurai

896. Electron/immuno-electron tomography of autophagosomal membranes and bacterial multidrug efflux systems. **M. Hayashi-Nishino**, K. Nishino

Hawaii Convention Center
307AB

Structure and Spectroscopy of Linear Polyenes: Finite and Infinite (#456)

Organized by: B. Hudson, N. Hush, T. Kobayashi, Y. Weng, J. Paldus, R. Christensen

Presiding: B. Hudson

8:00 – 897. Energetics and dynamics of the low-lying electronic states of constrained polyenes: Implications for infinite polyenes. **R. Christensen***, M. Enriquez, N. Wagner, A. Peacock-Villada, C. Scriban, R. Schrock, T. Polivka, H. Frank, R. Birge

8:30 – 898. Synthetic development of cyclopolymerization of 1,6-heptadiene derivatives and conformational study of polyene. **E. Kang**, T. Choi*

9:00 – 899. Cis-trans photoisomerization of 1,3,5-hexatrienes. **J. Saitiel***, C.E. Redwood, R. Samudrala, K. Laohhasurayotin,

9:30 – 900. Dissecting the photoinitiated dynamics of carotenoids in solution and in light harvesting proteins. **D.S. Larsen***

10:00 – 901. Single- and double-quantum 2D electronic spectroscopy refine the energy level scheme of carotenoids. **J. Hauer***

10:30 – 902. Singlet fission in carotenoid dimers and aggregates probed by time-resolved resonance Raman spectroscopy. **M.J. Tauber**

11:00 – 903. Nature of the intramolecular charge transfer (ICT) and forbidden ${}^1\text{B}_u^-$ states of peridinin and peridinin analogs. **N. Wagner***, J. Greco, M. Enriquez, H. Frank, R. Birge

Thursday Afternoon

Hawaii Convention Center
308A

Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44)

Organized by: S. Tretiak, G. Chen, Y. Tanimura
Presiding: Y. Tanimura

13:00 Opening remarks

13:05 – 904. Probing energy and charge transfer by broadband X-ray spectroscopy. **S. Mukamel**, J. Biggs, Y. Zhang, W. Hua

13:35 – 905. Nonlinear optical response in nanostructures induced by optical near-field. **K. Nobusada***

14:05 – 906. Simple and accurate method for time-dependent transport along nanoscale junctions. **L. Chen**, T. Hansen, I. Franco*

14:35 – 907. Decoherence in energy transfer dynamics from a mixed quantum-classical approach with the mapping formalism. **H. Kim**, Y. Rhee*

14:55 Break

15:10 – 908. First-principles method to simulate the dynamics of open electronic systems. **C. Yam**, G. Chen

15:40 – 909. Simulation of real-time electronic dynamics at molecule-bulk interfaces. **R. Wang**, X. Zheng*

16:10 – 910. Description of many-electron dynamics by multi-determinantal wave functions and reduced density matrices. **T. Kato***

16:40 – 911. Modeling of proton coupled electron transfer reactions in the framework of density functional theory . **U. Raucci***, N. Rega

Hawaii Convention Center
304A

Self-organization in Chemistry (#165)

Organized by: S. Nakata, J. Pojman, O. Steinbock, Q. Gao, J. Wang, T. Yamaguchi, R. Yoshida, S. Nakabayashi

Presiding: Q. Gao, I.Z. Kiss, S. Nakabayashi

13:00 – 912. Dynamics of networks of electrochemical oscillations. **I.Z. Kiss***, J. Coleman, Y. Liu, M. Sebek

13:30 – 913. Complex composite oscillations in the glucose-glucose oxidase-ferricyanide reaction under aerobic conditions. F. Mizuka, K. Ponomareva,

L. Schreiberova*, I. Schreiber

13:50 – 914. Exploring the collective behavior of redox polymer gels. **Z.A. Jimenez***, I.R. Epstein*

14:05 – 915. Application of oscillation in bacterial growth. **S. Sasaki**, M. Hosoki, H. Kato

14:20 coffee break

14:35 – 916. Multi-oscillator model of the circadian clock system and experiments: Why is eastbound long-distance trip so heavy? **H. Kori***

15:05 – 917. Cooperative phenomena in a set of nonlinear chemical oscillators. **A.P. Munuzuri***

15:25 – 918. Synchronization patterns in reactive dynamical chemical systems. **E. Panagakou**, N.M. Awal, I.R. Epstein*

15:40 – 919. Crowd synchrony in chaotic oscillators. **H. singh**, P. Parmananda

15:55 – 920. Synthesis of silica-supported cadmium oxide and phosphorescent zinc sulfide precipitation tubes using nonequilibrium processes. **J.J. Pagano**

16:10 – 921. Macroscopic self-oscillation dynamics of plate-like crystals under continuous blue light irradiation. **T. Ikegami**, Y. Kageyama, S. Takeeda

16:20 Discussion

Hawaii Convention Center
310 Theatre

Recent Progress in Matrix Isolated Species (#199)

Organized by: T. Momose, Y. Lee, D. Anderson
Presiding: R. Hinde, T. Momose

13:00 – 922. Hydrogen atom reactions in solid parahydrogen. **M.E. Balabanoff**, F.M. Mutunga, **D.T. Anderson***

13:30 – 923. Laser spectroscopy of radicals, carbenes, and ions in superfluid helium droplets. **G.E. Doublyer***

14:00 – 924. Capture and characterization of an activated carbon dioxide molecule on a Ni(1) complex using cryogenic vibrational predissociation spectroscopy. **M.A. Johnson**

14:30 – 925. Infrared spectra of free radicals and protonated species isolated in solid para-hydrogen. **Y. Lee***

14:50 Break

15:00 – 926. Hydrogen activation via quantum mechanical tunneling. **S. Henkel**, M. Ertelt, **W. Sander***

15:30 – 927. Raman spectroscopy of noble-gas compounds in matrix environments: A hybrid quantum-classical simulation. **A. Nakayama**

16:00 – 928. Ab initio study of O_2H^+ : A tracer molecule in the interstellar medium?. **R. Hernandez***

16:15 – 929. Investigation on imidazolium ionic liquids and water molecules by matrix isolation infrared spectroscopy. **W. Sung**, D. Kim*

16:30 – 930. Infrared spectra of protonated ovadane ($\text{C}_{32}\text{H}_{15}^+$) and its neutral counterpart in solid para-hydrogen: Formation mechanisms and implication to unidentified infrared emission. **M. Tsuge**, Y. Lee

16:45 – 931. Infrared spectra of NgBeSO_2 ($\text{Ng} = \text{Ne, Ar, Kr, Xe}$) in noble-gas matrices. **X. Wang***

Hawaii Convention Center
306B

Metal Ions and Protein Functions: Theoretical Models and Applications (#202)

Organized by: Q. Cui, M. Meuwly, T. Allen, Y. Gao
Presiding: K.M. Merz

13:00 – 932. Modulation of metalloregulator unbinding kinetics for transcription regulation in living cells. **P. Chen***

13:40 – 933. Allosteric regulation of nucleosome core particle by transition metal anticancer drugs . **U. Rothlisberger***

14:20 – 934. Mechanistic structural view of ras biology. **R. Nussinov***, T.S. Chavan, H. Jang, L. Khavruskii, N. Tarasova, V. Gaponenko

15:00 Break

15:15 – 935. Accurate modeling of metal ions in aqueous solution. **K.M. Merz***

15:55 – 936. Valence bond based force field for hypervalent molecules. **M.H. Schmid**, C.R. Landis

16:35 – 937. Active site dynamical effects that affect the hydrogen transfer rate-limiting step in the catalysis of linoleic acid by soybean lipoxygenase-1 (SLO-1): Primary and secondary isotope studies constructed using a new rare-events sampling ab initio dynamics methodology. **S.S. Iyengar**

Hawaii Convention Center
313B

Single-molecule Fluorescence Imaging (#208)

Organized by: P. Chen, T. Majima, G. Cosa
Presiding: C.F. Landes, M. Roeffaers

13:00 Catalysis II

13:00 – 938. Super-resolution fluorescence and stimulated Raman microscopy study of acid mordenite zeolites. **M. Roeffaers***, A. Kubarev, K. Liu, J. Hofkens

13:25 – 939. Copper nanocatalysis of the "click" reaction. **J. Sciano***, M.R. Decar, S. Impellizzeri, M. Marin

13:50 – 940. Single-molecule and -particle fluorescence microscopy for organic chemistry and catalysis. **S. Blum**

14:15 – 941. Single-molecule chemical reaction reveals molecular reaction kinetics and dynamics. **W. Xu***

14:30 – 942. Enzymatic catalysis: Disentangling chemical and conformational steps. **I. Grossmann**, H. Aviram, G. Armony, A. Horovitz, H. Hofmann, **G. Haran**, D. Fass

14:45 Break

15:00 Molecule-surface and molecule-host interactions

15:00 – 943. Molecular transport at wet interfaces. **D. Schwartz***

15:25 – 944. Hit 'em where they ain't: Super-resolution imaging of porous nanomaterial. **C.F. Landes***

15:50 – 945. Anomalous diffusion of guest dyes in amorphous polymer solids as revealed by single molecule tracking. **H. Miyasaka**, Y. Taga, K. Hiratsuka, Y. Arai, S. Ito

16:15 – 946. Following single molecules to a better understanding of mass transport phenomena in organized 1D silica mesopores. **D.A. Higgins***, R. Kumarsinghe, S. Park, T. Ito

16:30 – 947. 3D single-molecule tracking of various dye molecules in polymer films. **K. Hiratsuka***, Y. Taga, S. Takei, D. Kitagawa, S. Kobatake, S. Ito, H. Miyasaka

16:45 – 948. Visualizing the function of surface-bound fluorescent molecular rotors. **J.A. Hutchison***, H. Ujii, J. Hofkens, A. Herrmann, K. Müllen

Hawaii Convention Center
301A

Fundamental Science of Photon and Electron Induced Surface Processes (#228)

Organized by: H. Petek, J. Zhao, Y. Matsumoto
Presiding: M. Feng

13:00 – 949. Probing ultrafast surface chemistry and catalysis using LCLS. **A. Nilsson**

13:40 – 950. Ultrafast dynamics of photoexcited insulators probed by time- and angle-resolved photoemission. **M. Wolf***

14:20 – 951. Active electrons carried by surface plasmons. **V.A. Apkarian***

15:00 Coffee break

15:00 – 952. Charge transfer excitons at van der Waals interfaces. **X. Zhu**

15:40 – 953. Electronic excitation at organic film/substrate interfaces. **T. Munakata***, T. Yamada

16:20 – 954. Dynamics of charge transfer processes at well-defined metal/organic interfaces. **U. Höfer***

Hawaii Convention Center
312

Interplay between Theory and Experiment in Catalytic Research (#277)

Organized by: M. Ehara, C. Cramer, S. Dai, C. Jones, T. Ziegler, T. Tsukuda

13:00 – 955. Metal clusters in catalysis: Opportunities and challenges. **T. Tsukuda***

13:20 – 956. Atomically precise gold and bimetal nanoclusters for catalysis. **R. Jin**

13:45 – 957. Metastable platinum clusters acting as a superior catalyst. **T. Imaoka***, K. Yamamoto

14:00 – 958. Bimetallic platinum nanoparticles as electrocatalysts: Determining structure-activity relationships using X-ray absorption spectroscopy. **P.N. Duchesne**, C. Deming, S. Chen, P. Zhang

14:15 Break

14:30 – 959. Theoretical investigation of the catalytic activities for Au cluster catalysts. **M. Okumura***

14:55 – 960. Metal clusters as catalysts: Experimental analysis underpinned by DFT calculations. **G.F. Metha***, G.G. Andersson*, V. Golovko*, T. Nakayama*, K. Kimoto*, J. Alvino, T. Bennett, H. Al Qahtani, B. Donoeva, R. Adnan, D. Ovoshchnikov, D. Anderson, R. Kler

15:20 – 961. Size and support effects in catalysis by supported size-selected clusters. **S. Vajda**

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15:35 – 962. Reactivity of metal atoms and clusters on carbon surfaces: Insights from Reax simulations and DFT calculations. M. Mahmoodinia, **P. Astrand***, D. Chen
15:50 – 963. New insight into the mechanism of ammonia formation in the Haber-Bosch process. **A.L. Garden**, E. Skulason*
16:05 – 964. Supported M-salen catalysts for enantioselective reactions: Catalyst design, structure-reactivity trends, and reaction pathways. K. Venkatasubbaiah, M. Kennedy, C.D. Sherrill, **C. Jones**

Hawaii Convention Center
306A

Science with Beams of Radioactive Isotopes (#340)

Organized by: S. Yennello, K. Starosta, Y. Zhao, H. Haba
Presiding: X. Tang

13:00 – 965. Potential for harvesting of long-lived radioisotopes at the Facility for Rare Isotope Beams (FRIB): Synergistic activities for basic and applied nuclear science. **S.E. Lapi**, G.F. Peebles, A. Pen, B. Marois, N. Hubley, T. Mastren, S. Loveless, E. Bollinger, D.J. Morrissey
13:30 – 966. High-power target solutions for large-scale direct Tc-99m production via the Mo-100 ($p,2n$) reaction. S. Zeisler, K. Buckley, V. Hanemaayer, B. Hook, S. McDiarmid, M. Dodd, A. Cellier, J. Tanguay, X. Hou, J. Valliant, F. Prato, M.S. Kovacs, T. Ruth, F. Benard, P. Schaffer

14:00 – 967. Applications of nuclear science for nuclear security. **J.A. Cizewski***

14:30 – 968. Story of Miharu in response to the Fukushima Daiichi nuclear power plant accident. **T. Koike***, Y. Suzuki, S. Genyu, I. Kobayashi, H. Komori, H. Otsu, H. Sakuma, E. Sarasaud, K. Shimada, T. Shinozuka, H. Tamura, K. Tsukada, M. Urai, T. Yamamoto

15:00 Break

15:15 – 969. Simulating the supernova neutrinosphere with heavy ion collisions including neutron rich radioactive beams. **C. Horowitz***

15:45 – 970. Radioactive isotope beam developments at TRIUMF. **P. Kunz***, P. Briceault, J. Lassen, A. Teigelhofer, C. Andreo, F. Gracia

16:15 – 971. Beta-delayed neutron spectroscopy using trapped ions. **N. Scielzo***, A. Aprahamian, S. Caldwell, J. Clark, A. Czeszumka, S. Marley, E. Norman, S. Padgett, A. Perez Galvan, G. Savard, R. Segel, K. Sharma, K. Siegl, S. Strauss, B. Wang

16:40 – 972. Neutron generator facility at SFU - GEANT4 dose prediction and verification. **J. Williams***, K. Starosta

Hawaii Convention Center
305B

Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344)

Organized by: D. Kilin, S. Kilina, I. Burghardt, G. Scholes, U. Diebold, A. Selloni, X. Gong, Q. Sun, R. Asahi, K. Donnen
Presiding: F. De Angelis, S. Jensen

13:00 – 973. Sensitized photoinduced electron transfer across single crystal semiconducting oxide interfaces. **B.A. Parkinson***

13:30 – 974. Driving force of charge transfer at heterogeneous interfaces. **V. Vaissier**, M. Mavros, E. Hontz, T. Van Voorhis

13:55 – 975. On-the-fly fewest switches TD-DFT surface hopping method: Application to nonradiative relaxation in ZnO nanocrystals. X. Li, **D. Lingerfelt**

14:20 Break

14:30 – 976. Modeling organohalide perovskites for photovoltaic applications: From materials to interfaces. **F. De Angelis***

15:00 – 977. Recent progress in organometal halide perovskite solar cells. **N. Park***
15:30 – 978. From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics. **S. Tretiak**
16:00 – 979. Carrier dynamics of organic-inorganic metal halide perovskite semiconductors. **K. Yamashita***
16:30 – 980. Non-equilibrium real-time TDDFT and application to lead-halide perovskites. **J.A. Parkhill***, T. Nguyen, R. Nanguneri

Hawaii Convention Center
301B

Applications of Coherent Multidimensional Spectroscopy to Chemistry, Biology, and Materials (#370)

Organized by: W. Zhao, W. Zhuang, M. Cho, G. Sholes
Presiding: G. Scholes

13:00 – 981. Structure and excited state dynamics of electronically coupled molecular dimers in DNA by 2D fluorescence spectroscopy. **A.H. Marcus***

13:25 – 982. Molecular modeling of 2D electronic spectra and energy transfer dynamics in photosynthetic systems. C. Feng, **Y. Cheng***

13:50 – 983. 2D electronic-vibrational spectra: modeling correlated electronic and nuclear motion. F. Terenziani, **A. Painelli**

14:15 – 984. Mapping the nanoscale exciton diffusivity in heterogeneous electronically coupled materials with time-resolved super-resolution imaging. S.B. Penwell, L.D. Ginsberg, **N.S. Ginsberg***

14:40 – 985. Exploring coherent dynamics and electronic structure in porphyrin nanorings by 2D spectroscopy. V. Butkus, J. Alster, E. Basinskaite, R. Augulis, P. Neuhaus, L. Valkunas, H. Anderson, D. Abramavicius, **D. Zigmantas***

15:05 Break

15:20 – 986. Gaining insights into nanoaggregate structures of polycyclic aromatic hydrocarbons with 2D IR spectroscopy. **A. Krummel***, J. Cyran

15:45 – 987. Vibrational frequency fluctuation of ions in aqueous solutions studied by nonlinear infrared spectroscopy. M. Okuda, K. Ohta, **K. Tominao***

16:10 – 988. Hydration structure and dynamics of cyanoferrate anions revealed by ultrafast vibrational spectroscopy. **J. Wang***

16:35 – 989. Thermal denaturation of DNA studied by ultrafast 2D-IR spectroscopy. **N. Hunt***, G. Hithell, G. Greetham, M. Towrie, A. Parker, G. Burley, M. Baker

Hawaii Convention Center
305A

Practical Strategies for Modeling Non-Covalent Interactions (#372)

Organized by: G. Beran, Y. Jung, H. Nakai, J. Schmidt
Presiding: H. Nakai

13:00 – 990. Ab initio molecular crystal and liquid structure, spectra, and phase diagrams. **S. Hirata**

13:30 – 991. Embedding theories for chemical reactions in the condensed phase. **T.F. Miller**

14:00 – 992. Challenges of modeling three-body intermolecular interactions. **G. Beran***

14:20 – 993. Analysis of hydrogen bond energies and hydrogen bonding networks in water clusters using the locally projected molecular orbital perturbation theory. **D. Akase, M. Aida, K. Ohno, S. Iwata**

14:40 Break

14:50 – 994. Examining noncovalent interactions using modern computational approaches. **C. Corminboeuf***, P. de Silva, A. Prij, e. pastorcak

15:20 – 995. Fragment-based analysis of intermolecular interactions using fragment symmetry adapted perturbation theory (F-SAPT). **C.D. Sherrill**

15:50 – 996. Testing theoretical models of aromatic stacking and CH-pi interactions. **K.D. Shimizu***
16:10 – 997. Benchmark harmonic vibrational frequencies for hydrogen bonding in water clusters and explicitly hydrated systems. **G.S. Tschumper***
16:30 – 998. Accurate and efficient quantum chemistry methods for non-covalent interactions in many-body systems. **J. Herbert***

Hawaii Convention Center
304B

Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403)

Organized by: A. Amirfazli, Y. Zuo, J. Li
Presiding: A. Amirfazli, R. Miller, J.I. Siepmann

13:00 – 999. Comparative adsorption studies of surfactants at water/air, water/alkane vapor, and water/bulk alkane interface. A. Javad, N. Masic, E.V. Aksenenko, V.B. Fainerman, R. Miller*

13:30 – 1000. Determination of the way to make a Langmuir monolayer of particles at an air/aqueous interface whose stiffness is not reduced after collisions by foreign material. **C. McNamee**, H. Butt, M. Kappel

13:50 – 1001. Measurement of resonant vibrations of small sessile water droplets and its application to the determination of surface tension. **S. Yamashita***, K. Amano, N. Nishi, T. Sakka

14:10 – 1002. Determining surface and interfacial tensions with multiple drop and bubble configurations. **J. Yang, Y. Zuo***

14:30 – 1003. Water Repellent Coatings to Prevent Icing in Ski Lifts. F. Montes Ruiz-Cabello, M. Rodriguez-Valverde, A. Amirfazli, M. Cabrerizo-Vilchez*

14:50 Coffee Break

15:00 – 1004. Monte Carlo simulations of alkane/water/surfactant mixtures: Liquid-liquid equilibria and interfacial properties. **J.I. Siepmann**, D. Harwood, P. Bai, R. Lindsey, S. Warrag, C. Peters

15:25 – 1005. Spontaneous and forced resonance of liquid surface in micrometers-sized confined geometry. **A. Hibara***

15:45 – 1006. Metastable vapor in a Janus nanocontainer. **D. Bratko***, J.D. Driskill, D. Vanzo, S. Jables, A. Luzar

16:05 – 1007. Spreading of liquid Pb droplets on an Al surface exhibiting solid-liquid interfacial premelting. **B.B. Laird***, Y. Yang

16:25 – 1008. System size dependency analysis of homogeneous bubble nucleation by molecular dynamics. **M. Nakamura**, D. Suh, K. Yasuoka*

Hawaii Convention Center
307AB

Structure and Spectroscopy of Linear Polyenes: Finite and Infinite (#456)

Organized by: B. Hudson, N. Hush, T. Kobayashi, Y. Weng, J. Paludis, R. Christensen
Presiding: R. Christensen

13:00 – 1009. Linear conjugated polyenes: Extrapolation to the infinite chain limit. **B. Hudson***

13:30 – 1010. Photophysics and excited-state levels of some of linear polyenes. **T. Itoh***

14:00 – 1011. Ring-substituted diphenylhexatrienes: Controlling solid-state photoproperties by short alkyl chains. **Y. Sonoda**

14:30 – 1012. Photoinduced excited state dynamics and time-resolved spectroscopy of linear polyenes. **M.S. Schuurman***, S. Neville

15:00 – 1013. Annealing effect on the performance of P3HT:PCBM solar cells by ultrafast spectroscopy. Y. Wang, M. Chen, C. Lin, J. Fan, C. Chang, C. Liao, A. Yabushita, K. Wu, **T. Kobayashi***

15:30 – 1014. ESR spectroscopy of excited states in conducting polymers and their devices. **K. Marumoto**
16:00 – 1015. Application of polyene molecule as an interfacial probe for characterization of nanoparticulate TiO₂ surface property and protein*. **Y. Weng***
16:30 – 1016. Advances in conjugated polymers. **K. Akagi***
17:00 – 1017. On the cooperative effect of donor and acceptor substituents coupled through a polyene chain of various lengths. **P.A. Limacher***

Thursday Evening

Hawaii Convention Center
301B

Synergistic Relationships between Computational Chemistry and Experiment (#9)

Organized by: S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: G. DiLabio

19:00 – 1018. Professor Russell J. Boyd: A career of scientific distinction. **H.F. Schaefer***

19:20 – 1019. Arvi Rauk: Some scientific adventures. **L. Radom***

19:40 – 1020. Elucidation of complicated reactions around electrolyte – electrode interfaces in Li-ion battery. **Y. Tateyama***, K. Sodeyama, J. Haruyama

20:00 – 1021. Room-temperature ionic liquids at solid interfaces: A combined computational and experimental investigation. **D.M. Smith***

20:20 – 1022. Generalized energy-based fragmentation approach for structures and spectra of large molecules and molecular crystals. **S. Li**

20:40 – 1023. Computational study on CO₂ chemical absorption process: Thermodynamic and dynamic analyses. **H. Nakai**

Hawaii Convention Center
Halls I, II, III

Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44)

Organized by: S. Tretiak, G. Chen, Y. Tanimura

Poster Session

19:00 – 21:00

1024. Molecular modeling and structural analysis of two-pore domain potassium channels TASK-1 interacting with the blocker A1899. **D.M. Ramirez**, B.a. Arevalo, G. Martinez, N. Decher, W. Gonzalez

Hawaii Convention Center
Halls I, II, III

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: A. Bertram, E. Bieske, A. Laskin, S. Nizkorodov, C. Ro, X. YANG

* Principle Author

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Poster Session

19:00 – 21:00

- 1025.** Online hygroscopicity and chemical measurement of urban aerosol in Shanghai, China. **X. YANG**
- 1026.** Photolysis of secondary organic aerosol material as a source of small oxygenated volatile organic compounds. **K. Malecha**, S. Nizkorodov*
- 1027.** Aqueous photochemical aging and molecular-level characterization of secondary organic aerosol using high-resolution mass spectrometry. **D. Romanosky***, J. Laskin, A. Laskin, S. Nizkorodov
- 1028.** Viscosity and diffusion in organic particles. M. Song, J.W. Grayson, Y. Chenyakin, P. Liu, Y. Zhang, S. Kamal, S. Martin, A. Bertram
- 1029.** Chemical composition of PM_{2.5} and VOC emissions from household cookstoves in Palwal District, Haryana, India. **L.T. Fleming**, S. Nizkorodov*, D.R. Blake, R.D. Edwards, P. Lin, A. Laskin, J. Laskin, K.R. Smith, N.K. Arora, M. Vaswani
- 1030.** Effects of humidity, NO_x, and ammonia on the optical properties and molecular composition of photo-oxidized naphthalene secondary organic aerosols. **P.K. Alona**, A. MacMillan, J. Lee, X. Zhang, T. Helgestad, G. Novak, P. Lin, V. Perraud, J. Laskin, A. Laskin, T. Bertram, C. Cappa, S. Nizkorodov*
- 1031.** Size-segregated analysis of ionic composition of aerosols transported from East Asia to Cape Hedo, Okinawa through Kumamoto City. **S. Tatsuta**, K. Shimada, A. Yoshino, A. Takami, S. Hatakeyama*
- 1032.** Long term and seasonal variation of carbonaceous aerosols in Okinawa, Japan. **Y. Taniguchi**, K. Shimada, A. Fusihini, A. Takami, S. Hatakeyama*
- 1033.** Hydrogen peroxide produced by carbonaceous particles in physiologically relevant medium. D. Hinz, J. Barnes, C. Gutierrez, **A.M. Johansen***
- 1034.** Liquid chromatography separation of brown carbon constituents produced in methylglyoxal-ammonium sulfate mixtures. **P. Lin***, J. Laskin, A. Laskin
- 1035.** Characterization of Antarctic sea-salt aerosols collected at King George Island by the combined use of low-Z particle EPMA, Raman microspectrometry, and ATR-FTIR imaging. **H. Eom***, H. Cho, H. Hwang, S. Hur, Y. Gim, D. Gupta, C. Ro*
- 1036.** Volatilization of acid from levitated single aerosol droplet in air studied by laser trapping-microspectroscopy. **A. Miura**, A. Horii, N. Kitamura
- 1037.** Investigation of chemical compositions of urban haze aerosols at Shanghai and Taiyuan, China using low-Z (atomic number) particle electron probe X-ray microanalysis. **H. Geng***, H. Zhou, Y. Zhang, R.J. Zeng, Y. Song, L. Wu, C. Ro
- 1038.** Sea salt aerosols as a reactive surface for inorganic and organic acids in the arctic troposphere. **J. chi**, Y. Zhang, **w. li***
- 1039.** Single-particle characterization of aerosols collected at Baengnyeong Island by low-Z particle EPMA. **H. Hong***, D. Gupta, A. Malek, H. Jung, H. Geng, C. Ro*
- 1040.** Source identification of particulate matters in an industrial city. S. Lee, J. Cho, **S. Choi***
- 1041.** Prediction of spatial and seasonal distributions of particulate polycyclic aromatic hydrocarbons using passive air samplers and gas/particle partitioning models. **S. Kim***, H. Kwon, M. Park, S. Choi
- 1042.** Size distribution and chemical composition of particulate matters in the multi-industrial city of Ulsan, Korea. **M. Park***, S. Kim, Y. Gim, H. Kwon, S. Choi
- 1043.** Microfluidic system for bioaerosol analysis. W. Jing, L. Zheng, S. Liu, **G. Sui**
- 1044.** Laser trapping and spectroscopy of single supercooled water droplets in air. **S. Ishizaka***, A. Oomae, T. Fujiwara

- 1045.** Determination of accurate vibrational line shapes and decoherence lifetimes of α -pinene using high-resolution broadband sum frequency generation (HR-BB-SFG) spectroscopy. **A.L. Mifflin***
- 1046.** Laser trapping and fluorescence correlation spectroscopy for the study on viscosity of single supercooled water droplets in air. **T. Ishikawa**, T. Fujiwara, S. Ishizaka*
- 1047.** Laser trapping of black carbon particles in air with a single focused laser beam. **M. Uraoka**, T. Fujiwara, S. Ishizaka*
- 1048.** Aerosol formation of water on solid seeds by molecular dynamics. **D. Suh**, K. Yasuoka
- 1049.** Organic speciation and source investigation of atmospheric fine particulate matter in the Pearl River Delta region. **X. Huang**, T. Zhang, Y. Feng, Q. Zhang, J. Yu*
- 1050.** Characterization of ambient aerosols from Amazonian rainforest and city of Manaus, Brazil. **L. Wu***, X. Li, H. Eom, D. Gupta, H. Chae, R. Godoi, C. Ro*
- 1051.** Molecular characterization of organic content of soot along the centerline of a coflow diffusion flame. J. Cain, **A. Laskin**, M. Khogly, M. Thomson, H. Wang
- 1052.** Change of organic composition with atmospheric condition in PM 2.5 and TSP collected at urban and non-urban sites. **J. Lee***, Y. kim, C. Jung, P. Lin, J. yu, J. kim
- 1053.** Hygroscopic properties and aqueous phase chemical reaction of micrometer-sized NaCl-malonic acid mixture aerosol particles. **X. Li***, D. Gupta, G. Park, J. Lee, C. Ro*

Hawaii Convention Center
313C**Recent Progress in Molecular Theory for Excited-state Electronic Structure and Dynamics (#142)**Organized by: J. Hasegawa, M. Collins, M. Gordon, P. Piecuch, T. Taketsugu
Presiding: J. Hasegawa

- 19:00 – 1054.** Excited-state multiple proton transfer reactions of 7-azaindole with methanol, water, and ammonia clusters in the gas phase: Molecular dynamics simulations. **N. Kungwan***

- 19:20 – 1055.** Excited state ab-initio molecular dynamics to model the green fluorescent protein photo-induced reactivity. **G. Donati***, A. Petrone, P. Cimino, N. Rega*

- 19:40 – 1056.** Ab-initio molecular dynamics combined with different solvation models for simulating excited state proton transfer. **U. Raucci***, N. Rega*

- 20:00 – 1057.** Moving past the particle-hole description of excited states: Affordable methodologies. **D.B. Williams-Young***, W. Yang, X. Li

- 20:20 – 1058.** Evaluating Δ SCF-like strategies for efficient exploration of excited state potential energy surfaces. **K. Komoto**, V. Laszlo, T. Kowalczyk

- 20:40 – 1059.** Transition properties in X-ray spectroscopy. **P.J. Lestrance***, X. Li

Hawaii Convention Center
Halls I, II, III**Self-organization in Chemistry (#165)**Organized by: S. Nakata, J. Pojman, O. Steinbock, Q. Gao, J. Wang, T. Yamaguchi, R. Yoshida, S. Nakabayashi
Presiding: S. Nakata, O. Steinbock, J. Wang**Poster Session**
19:00 – 21:00

- 1060.** Studies of micellization of dodecyltrimethylammonium bromide-sodium decyl sulphate in pure water and methanol-water mixed solvent media. **A. Bhattacharai***

- 1061.** Self-propelled oil droplet chasing pH wave-front propagation. **N. Magome***, H. Sakuta, T. Okuda, N. Umezawa, Y. Mori, K. Yoshikawa
- 1062.** Batch oscillations in the acidic peroxide-bromide system. **G. Frerichs**
- 1063.** Dynamic responses of an amphiphilic molecular layer to chemical stimuli. **A. Deguchi**, Y. Seki, K. Fukuhara, N. Kumazawa, S. Nakata
- 1064.** Characteristic motion and mode-bifurcation of a self-propelled motor on water depending on the physico-chemical environment. **M. Yoshi***, Y. Matsuda, N.J. Suematsu, S. Nakata
- 1065.** Coexistence and transition of precipitation wave and stationary Liesegang rings. **J. Zheng***, C. Pan*, L. Ren, Q. Gao*
- 1066.** Synchronization patterns of a reduced coupled Oregonator model using piecewise linear approximation. **N.M. Awal**, E. Panagakou, I.R. Epstein*
- 1067.** Self-assembly behavior of mixed surfactants at interfaces. **Y. Li***, Y. Sun, Y. Zhang, Q. Deng, H. Sun
- 1068.** Rebirth of dead oscillator in Ferroin-catalyzed BZ reaction. **Y. Unegi**, M. Minato, H. Sawahata*
- 1069.** I-F relationship and light-driven directional movement of self-oscillating gel. **L. Ren***, H. Luo, I.R. Epstein, Q. Gao
- 1070.** Novel micromotor working under stationary DC electric field. **S. Mori***, T. Kurimura, M. Miki, D. Yamamoto, A. Shioi, K. Yoshikawa
- 1071.** Continually propagating chemical pathway responds to environmental changes. **M. hardy**
- 1072.** Application of oscillation in bacterial growth. **M. Hosoki***, S. Sasaki
- 1073.** Optochemically organized filaments of light: From waveguide encoded intersecting (WIDEI) polymer lattices to spontaneous, all-optical transfer of signals. **K. Saravananmuttu**, H. Lin, I. Hosein, A. Hudson, D. Basker, M. Ponte
- 1074.** Escaping liquid-droplet against unfavorable gas stimulus: Self-propelling motion driven by interfacial instability. **H. Sakuta***, N. Magome, Y. Mori, K. Yoshikawa
- 1075.** Network motifs and mechanisms for oscillatory dynamics of enzyme reactions. F. Muzika, D. Denisov, V. Radovicov, L. Schreiberova, M. Pribyl, I. Schreiber*
- 1076.** Behaviors of the Belousov-Zhabotinsky reaction system in the presence of acrylic monomers. **Y. Furue**, T. Banno, K. Asakura
- 1077.** Collective motion of intermittent camphor boats. **T. Ichino**
- 1078.** "Surface-inactive" effect induced by adding nonionic surfactants on a mixture of water and organic solvent. **M. Hachiya**, K. Sadakane, K. Fukao
- 1079.** Numerical experiments of surface and bulk flow emerging with single chemical wave propagation in Belousov-Zhabotinsky reaction. **A. Nomura***, T. Sakurai, H. Miike
- 1080.** Construction of vesicular system containing catalyst-producing system. **K. Kurihara***, L. Sheng
- 1081.** Giant vesicle containing a photosensitive smaller giant vesicle. **K. Machida**, K. Suzuki, T. Sugawara, K. Yamaguchi
- 1082.** Self-emergence of spatial order on number of standing objects with the time-development through reentrant bifurcation, stationary-fluctuation-stationary: Experiment with vibrating plate. **S.I. Takatori***, T. Ichino, K. Yoshikawa
- 1083.** Lifetime of a Turing pattern generated by the CIMA reaction in an open gel reactor composed of alkyl ammonium cat-ionic side chains. **Y. Miyazaki**, T. Banno, K. Asakura*
- 1084.** Conformation change and odd/even effect observed in Langmuir layer of anthraquinone derivative at liquid-air interface. **Y. Tamaki***, A. Honda, Y. Takahashi, K. Miyamura
- 1085.** Time-development of spatial ordering from circular pearling to 2D hexagonal packing through a 1D linear array of emerging droplets. **D. Yamamoto**, A. Shioi, M.P. Kraft, K. Yoshikawa

- 1086.** Navigation speed of a camphor boat on bubbly water. **M. Shimokawa**, R. Egashira
- 1087.** Morphological diversity of giant vesicle-based protocell depending on degree of complexation of DNA and catalysts. **M. Matsuo**, K. Kurihara, T. Toyota, T. Sugawara

- 1088.** Standing thin-film formation of the rotator phase of perfluoroborate with wet process. **S. Tanaka***, F. MUHAMMAD, A. Taguchi, H. Honda
- 1089.** Colloidal ordering and membrane deformation in giant vesicles encapsulating two kinds of particles. **Y. Natsume***, K. Ito, K. Kurihara
- 1090.** Self-inverted reciprocation of an oil droplet on a surfactant solution. **S. Nakata**, Y. Sogabe, S. Tanaka

Hawaii Convention Center
310 Theatre**Recent Progress in Matrix Isolated Species (#199)**Organized by: T. Momose, Y. Lee, D. Anderson
Presiding: M.S. Gudipati

- 19:00 – 1091.** Spectroscopy of isolated amino acids and amino acid-water complexes. **G. Tarçay**, G. Bázso, E. Najbauer, G. Magyarfalvi

- 19:30 – 1092.** Infrared spectroscopy of peptides and proteins embedded in helium droplets. **G. von Helden***

- 20:00 – 1093.** Chiroptical spectral signatures of flexible chiral molecules and their hydrogen-bonded clusters in cold matrices. A. Perera, C. Merten, J. Thomas, Y. Xu*

- 20:30 – 1094.** First observation of the elusive triazine molecule (N₃H₃). **M. Förstel***, P. Maksyutenko, R. Kaiser

- 20:45 – 1095.** Infrared spectroscopy of amino acids in parahydrogen matrices. **T. Momose***

Hawaii Convention Center
306B**Metal Ions and Protein Functions: Theoretical Models and Applications (#202)**Organized by: Q. Cui, M. Meuwly, T. Allen, Y. Gao
Presiding: Y. Gao

- 19:00 – 1096.** Electron flow through biological molecules. H.B. Gray, **J.R. Winkler***

- 19:40 – 1097.** Redox-driven proton pumps: Insights from computer simulations. **A.A. Stuchebrukhov***

- 20:20 – 1098.** Molecular dynamics simulation of enzyme-catalyzed reactions with metal cofactors. **J. Gao**

Hawaii Convention Center
Halls I, II, III**Single-molecule Fluorescence Imaging (#208)**

Organized by: P. Chen, T. Majima, G. Cosa

* Principle Author

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Poster Session

19:00 – 21:00

1099. Single molecule perspective on mass transport over chemically graded self-assembled monolayers. **D.A. Higgins**, D. Giri*, K. Ashraf, M.M. Collinson

Hawaii Convention Center
301A

Fundamental Science of Photon and Electron Induced Surface Processes (#228)

Organized by: H. Petek, J. Zhao,
Y. Matsumoto
Presiding: M. Kawai

19:00 – 1100. STM tip-induced reaction of methanol on TiO₂ (110) surface. s. Tan, H. Feng, y. Ji, **B. Wang***, Q. Zeng, Y. Shi, J. Zhao, A. Zhao, Y. Luo, J. Yang, J. Hou
19:40 – 1101. Reversible reactions of methanol on rutile TiO₂(110) mediated by proton transfer. **S. Tan**, Q. Zheng, H. Feng, J. Zhao*, B. Wang, X. Cui*

20:00 – 1102. Advanced modeling of heterogeneous photocatalysis: From ground-state quasiparticle level alignment to photoreaction mechanism. **A. Migani***
20:20 – 1103. On the mechanism of heterogeneous photocatalysis under magnetic field. **H. OKUMURA***, S. Endo, E. YAMASUE, K.N. Ishihara

20:40 – 1104. Evaluation of energy-resolved density of electron traps in particulate photocatalysts by reversed double-beam photoacoustic spectroscopy. **A. Nitta***, M. Takase, B. Ohtani

Hawaii Convention Center
305B

Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344)

Organized by: D. Kilin, S. Kilina, I. Burghardt, G. Scholes, U. Diebold, A. Selloni, X. Gong, Q. Sun, R. Asahi, K. Domnen

19:00 introducing remarks
19:01 Dynamics and Charge Transfer at interfaces
19:01 – 1105. In-situ evaluation of photocatalytic carriers on TiO₂/liquid interface with the transient grating method.
S. Kuwahara, K. Katayama

19:16 – 1106. Experimental and theoretical studies on transient kinetics of carriers in LaTiO₂N solid photocatalyst affected by trap states. **K. Seki**, Y. Suzuki, A. Furube, R. Singh, H. Matsuzaki, T. Minegishi, T. Hisatomi, K. Domnen

19:31 – 1107. Theoretical study of charge transfer type excitons at donor/acceptor interfaces of organic solar cells.
A. MURAOKA, M. Fujii, K. Mishima, R. Jono, K. Yamashita

19:46 – 1108. Electron injection mechanism of squaraine-based sensitizers adsorbed on a TiO₂ cluster in dye-sensitized solar cells: A DFT/TDDFT investigation. **C. Tan**, H.G. Tsai

20:01 – 1109. Titanium hydroxide and polyoxotitanate clusters: A nanostructure comparison. **D.J. Vogel**, D. Kilin*

20:15 Photocatalytic Reactions

20:15 – 1110. FT-IR and mass spectroscopic investigation of photochemistry of mesoporous nanomaterial. **D. Paul***

20:30 – 1111. CO₂ reduction under periodic illumination of ZnS. **R. Zhou**, M.I. Guzman*

Hawaii Convention Center
Halls I, II, III

Practical Strategies for Modeling Non-Covalent Interactions (#372)

Organized by: G. Beran, Y. Jung, H. Nakai, J. Schmidt

Poster Session

19:00 – 21:00

1112. Correcting for basis set superposition error on reactive potential energy surfaces. **M. Gutowski***, S.G. Escher, A. Whitesides

1113. Synergistic effect of B...N coordinate bonding and ring strain makes 2-APB an ideal drug with dual effect. **H. Dong***, W. Li, J. Sun, S. Li, M.L. Klein

1114. Molecular mechanisms of ZnO nanoparticle dispersion in solution: Modeling of surfactant association, electrostatic shielding, and counter ion dynamics. **P. Duchstein***, T. Milek, D. Zahn

1115. Reverse-docking and virtual screening of asymmetric organocatalysts. **G. Deslongchamps***

1116. Comparative investigation of the non-covalent binding of nonsteroidal anti-inflammatory drugs with the active site of cyclooxygenase isoforms. F. Akcasal*, P. Aksu, **Türkay**, A. Dimoglo

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable, K. Liu, J. Lane, Y. Kajii, X. You
Presiding: D. Osborn

19:00 Opening Remarks

19:02 – 1117. Keto-enol photo-tautomerization is responsible for the formation of organic acids in the atmosphere. M. Shaw, A. Kharazmi, B. Szczaray, L. Whalley, D. Heard, D. Osborn, M. Jordan, S. Kable*

19:32 – 1118. Formation and oxidation mechanism of atmospheric enols. **G. da Silva***

20:02 – 1119. Using the master chemical mechanism as a framework to explore the impacts of newly discovered chemical processes on atmospheric composition and oxidising capacity. **L. Whalley***, D. Heard, R. Hansen, M. Blitz, P. Seakins, T. Ingham, S. Kable, M. Jordan, M. Shaw, D. Osborn, B. Szczaray, C. Fittschen

20:22 – 1120. Atmospheric chemistry of short-chain haloolefins. **T.J. Wallington***, M. Andersen, O.J. Nielsen

20:42 Poster Slam

Hawaii Convention Center
307AB

Developments in Spectroscopic Investigation of Intermolecular Interactions and Dynamics of Molecular Clusters (#438)

Organized by: H. Sekiya, T. Zwier, M. Fujii, E. Bieske, N. Kim
Presiding: E. Bieske

19:00 – 1121. Mechanism of the ionization induced isomerization of phenol-Ar cluster studied by mass analyzed threshold ionization detected infrared spectroscopy. **M. Miyazaki**, K. Müller-Dethlefs, O. Dopfer, M. Fujii*

19:20 – 1122. On the Stark effect in open shell complexes exhibiting partially quenched electronic angular momentum. **G.E. Douberly***, C.P. Moradi

19:40 – 1123. Cooperative effects on hydrogen-bonded networks in molecular clusters and crystals studied via vibrational spectroscopy and quantum chemical calculations. **H. Sekiya***

20:05 – 1124. Electronic circular dichroism spectroscopy of chiral molecules and clusters in a supersonic jet. **N. Kim***

20:30 – 1125. Effect of aromatic molecules on the spectroscopy and structure of water clusters. E.G. Buchanan, P.S. Walsh, D.P. Tabor, E.L. Sibert, **T.S. Zwier**

20:55 Closing Remarks

Hawaii Convention Center
Halls I, II, III

Structure and Spectroscopy of Linear Polyenes: Finite and Infinite (#456)

Organized by: B. Hudson, N. Hush, T. Kobayashi, Y. Weng, J. Paldus, R. Christensen

Presiding: R. Christensen, B. Hudson, T. Kobayashi

Poster Session

19:00 – 21:00

1126. Necessary lack of bond alternation in polyacetylene. **B. Hudson**

1127. Excited electronic states and spectroscopy of methylphenylpolyenes. **T. Itoh***

1128. Resonant Raman and infrared absorption studies of isolated and conjugated polyene chains embedded in a urea inclusion complex. **S.A. Dinca**, D. Allis, M.B. Sponsler, B. Hudson

1129. Electronic absorption spectra and photophysics of diiodo linear polyenes and photopolymerization of α,ω -diiodoalkanes in host urea inclusion compounds. **P.F. McLaughlin**, B. Hudson

Friday Morning

Hawaii Convention Center
301B

Synergistic Relationships between Computational Chemistry and Experiment (#9)

Organized by: S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim

Presiding: A. East, H.F. Schaefer

8:00 Statistical fluctuations, dynamics, and de novo enzyme catalysis. **T. HeadGordon***

8:20 – 1131. In silico prediction of pharmaceutical degradation pathways: A Zeneth benchmarking study. **D.L. Reid***

8:40 – 1132. Computational studies of catalytic reactions of organic molecules, enzymes, and metal-organic frameworks. **H. Hira***

9:00 – 1133. Quantum-chemical structure optimization of biomolecules: are the popular methods really the best possible choice? **L. Goerigk***

9:20 – 1134. SP Explorer: Novel software facilitating the exploratory analysis of chemical simulations. **K.W. Hall***, C. Hurter, S. Carpendale, P.G. Kusalik

9:40 Break

9:50 – 1135. Antiaufbau electron configurations in DNA. **G. Jiande***, M.L. Coote

10:10 – 1136. Impact of bulky carcinogens on DNA structure and function. **S. Wetmore**

10:30 – 1137. DNA damage by aristolochic acids and ochratoxin A: A tale of two toxins. **P. Sharma**

10:50 – 1138. Hierarchical multiscale study of DNA structure and dynamics. **A. Laaksonen***

11:10 Break

Hawaii Convention Center
308A

Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44)

Organized by: S. Tretiak, G. Chen, Y. Tanimura
Presiding: G. Chen

8:00 Opening Remarks

8:05 – 1139. Bottom-up excitonics. **A. Aspuru-Guzik***

8:35 – 1140. Computational studies of energy transfer in dendrimers. **A.E. Roitberg***

9:05 – 1141. Theoretical studies on triplet-triplet annihilation processes of diphenylanthracene derivatives in solution. **Y. Shigeta***

9:35 – 1142. Ultrafast electron-hole dynamics in dinaphtho[2,3-b:2',3']thieno[3,2-b]thiophene (DNTT) organic semiconductor. **T. Fujita***, S. Atahan-Evrak, N. Sawaya, A. Aspuru-Guzik

9:55 Break

10:10 – 1143. Quantum simulation of coherent exciton dynamics in conjugated systems. **P.J. Rossky***

10:40 – 1144. Understanding and tuning excitons of organic materials. **L. Wang**

11:10 – 1145. Theoretical study on photoinduced charge transfer at molecular interfaces. **K. Yamashita**

11:40 – 1146. Ground and excited state ab initio molecular dynamics with non periodic boundary conditions to model charge transfer processes in condensed phase. **N. Rega***

Hawaii Convention Center
313B

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, O. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: S. Nizkorodov, C. Ro

8:00 opening remarks

8:05 – 1147. Water uptake and heterogeneous chemistry of authentic and model sea spray aerosol particles. **V. Grassian***

8:35 – 1148. Evidence for biological and photochemical seawater influence on sea spray aerosol water soluble and water insoluble organic matter composition revealed by ultrahigh resolution mass spectrometry. **A.S. Wozniak**, A. Willoughby, S. McElhenie, P.K. Quinn, D.J. Coffman, P.G. Hatcher

8:50 – 1149. Hygroscopic behavior of NaCl-MgCl₂ mixture particles as nascent sea spray aerosol surrogates including dynamic structural rearrangement in MgCl₂ hydrates. **D. Gupta**, H. Eom, H. Cho, J. Lee, C. Ro*

9:05 – 1150. Humidity-dependent surface tension measurements of individual sub-micrometer liquid particles. **A.V. Tivanski**

9:20 – 1151. Atmospheric particles: Viscosity, phase, and response to relative humidity. **M.K. Gilles***, T.H. Harder, B. Wang, R.E. O'Brien, S. Nizkorodov, A. Laskin

9:50 Break

10:00 – 1152. Insights into atmospheric ice nuclei from laboratory and field measurements. D. Haga, R. Mason, R. Iannone, M. Wheeler, C. Chou, V. Irish, M. Si, R. Dickie, **A. Bertram**, C.L. Schiller, J.P. Abbott, J.A. Huffman, J. Li

10:20 – 1153. Imaging the interiors of individual aerosol particles using transmission electron microscopy. **K. Adachi***, P.R. Buseck

10:50 – 1154. Physical state of the atmospheric particle population above a tropical rain forest in GoAmazon2014/5. **S. Martin***, A. Bateman, R. Souza, P. Artaxo

11:10 – 1155. Molecular characterization and chemical imaging of atmospheric organic particles collected in the Amazonia. **A. Laskin***, J. Laskin, P. Lin, B. Wang, A.B. Guenther, P. Artaxo, S. Nizkorodov, R. O'Brien, M.K. Gilles

* Principle Author

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onlineprogram

11:30 – 1156. Aerosol physical and chemical properties in Amazonia investigated in the GoAmazon 2014/15 experiment.
P. Artaxo, H. Barbosa, S. Carbone, J.F. Brito, B. Holanda, G. Cirino, R. Souza, L. Rizzo, S.T. Martin, M.O. Andreae

Hawaii Convention Center
308B

Advances in Quantum Monte Carlo (#80)

Organized by: S. Tanaka, L. Mitas, P. Roy
Presiding: P. Roy

8:00 – 1157. Approach to pure-sampling quantum Monte Carlo. **S. Rothstein***

8:30 – 1158. Exact QMC calculations for the H-H-H system using flexible single-determinant trial functions. **J.B. Anderson***

9:05 – 1159. How do exact quantum Monte Carlo projection methods behave in the thermodynamic limit? **D. Ceperley***, M. Holzmann

9:40 – 1160. It's NO MAGIC: A new method for electronic structure theory that uses compressed sensing and imaginary time evolution. **A. Aspuru-Guzik***

10:05 Break

10:15 – 1161. Window on universality through simulations of entanglement entropy. **R.G. Melko***

10:50 – 1162. Entanglement in quantum fluids and gases. **A. Del Maestro***

11:25 – 1163. Using quantum Monte Carlo to study magnetism, delocalization, and electronic correlation in materials. **L.K. Wagner**

Hawaii Convention Center
304A

Self-organization in Chemistry (#165)

Organized by: S. Nakata, J. Pojman, O. Steinbock, Q. Gao, J. Wang, T. Yamaguchi, R. Yoshida, S. Nakabayashi
Presiding: A. De Wit, H. Kitahata, N.J. Suematsu

8:00 – 1164. Liesegang patterns of calcium carbonate and calcium phosphate in various gel medium. **A. Kamimaga***, J. Kurawaki

8:15 – 1165. Pattern formation in reactive flows. **A. De Wit***

8:45 – 1166. Oscillatory motion of self-propelled Belousov-Zhabotinsky droplet. **N.J. Suematsu***, K. Ito, T. Amemiya, Y. Mori, S. Nakata

9:05 – 1167. Spontaneous interfacial convection and the corresponding electrical potential oscillation in three-phase liquid membrane system. **B. Nanzai***, D. Terashita, Y. Koyano, H. Kitahata, M. Igawa

9:25 – 1168. Division of self-propelled oil droplet induced by amphiphilic precursor. **T. Banno**, K. Asakura, T. Toyota*

9:40 coffee break

9:55 – 1169. Self-propelled nanomotors and nonlinear chemical dynamics. **R. Kapral**, B. Robertson

10:25 – 1170. Blebbing motion of an oil-water interface induced by transition of lamellar structure. **Y. Sumino***, N. Yamada, M. Nagao, H. Kitahata, Y. Melnichenko, H. Seto

10:45 – 1171. Oscillatory dynamics of active deformable particles. **M. Tarama***, T. Ohta

11:00 – 1172. Spontaneous movement of oil-droplet emerged after photochemical reaction. **K. Suzuki***, N. Nakayama, T. Sugawara*

11:15 – 1173. Theoretical approach to congestion of camphor boats. **K. Ikeda***, S. Ei, M. Nagayama, A. Tomoeda

11:30 Discussion

Hawaii Convention Center
310 Theatre

Recent Progress in Matrix Isolated Species (#199)

Organized by: T. Momose, Y. Lee, D. Anderson
Presiding: Y. Lee, W. Sander

8:00 – 1174. Molecular reactions on water and ice media. **B.R. Gerber**

8:30 – 1175. Matrix-isolation in water-ice: Applications to chemistry, astrophysics, and planetary sciences. **M.S. Rudipati**

9:00 – 1176. Irradiation of N₂-dominated ices relevant to Triton and Pluto. **Y. Wu***

9:30 – 1177. Kuiper Belt objects: A case study of matrix isolated species on the macroscopic scale. **R. Kaiser**

10:00 Break

10:15 – 1178. Nuclear spin conversion of H₂O in rare gas matrices. **J. Vermette, P. Turgeon***, P. Ayotte, X. Michaut

10:30 – 1179. Low temperature studies of halogenated reaction intermediates: From iso-halocarbons to radical-molecule complexes. **S.A. Reid**

11:00 – 1180. Matrix isolation spectroscopic studies of coronene reactions with water and iron: New insights in astrochemistry of neutral PAHs. **J. Mascetti**, J.A. Noble*, A. Moudens, C. Aupetit

11:30 – 1181. Electronic spectroscopy of mass-selected hydrocarbon ions and radicals in neon matrices. **J.P. Maier**

Hawaii Convention Center
306B

Metal Ions and Protein Functions: Theoretical Models and Applications (#202)

Organized by: Q. Cui, M. Meuwly, T. Allen, Y. Gao
Presiding: M. Meuwly

8:00 – 1182. Artificial metalloenzymes: Challenges and opportunities. **T.R. Ward**

8:40 – 1183. Force field-based simulations of metal-containing systems. **M. Meuwly***

9:20 – 1184. Metalloenzymes from quantum many-body wavefunctions. **G.K. Chan**

10:00 Break

10:10 – 1185. Ab initio QM/MM molecular dynamics simulations of zinc-dependent histone deacetylases. **Y. Zhang**

10:50 – 1186. QM/MM calculations of reactions in proteins. **U. Ryde***

11:30 – 1187. Understanding metalloenzyme catalysis with QM/MM free energy simulations. **Q. Cui***

Hawaii Convention Center
Halls I, II, III

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Eikerling, G. Jerkiewicz, S. Mitsuhashima, A. Gewirth

Poster Session

10:00 – 12:00

1188. Theoretical study of the prediction of the electronic and inhibition properties of Schiff base (E)-2-(4-hydroxybenzylideneamino) phenylarsonic acid.

M. Castro*, M.J. Percino, M. Cerón, J. Soriano, V. Chapela, O. Rodríguez

1189. Morphology-controlled synthesis of platinum-based nanocrystals and their electro-catalytic activities toward oxygen reduction reaction. **Y. Li***, F. Quan, L. Chen

1190. CO₂ electroreduction over Cu and Au nanostructured catalysts: Size, oxidation state, and interparticle distance effects.

H. Mistry, R. Reske, F. Behafarid, P. Strasser, **B. Roldan Cuenya***

1191. Influence of surface charges at insulating materials on the voltammetric behavior of nanoelectrodes. **C. Kubel***, A. Bund

Hawaii Convention Center
301A

Fundamental Science of Photon and Electron Induced Surface Processes (#228)

Organized by: H. Petek, J. Zhao, Y. Matsumoto
Presiding: V.A. Apkarian

8:00 – 1192. Electron transport through a single molecule and the excitation observed by STM. **M. Kawai***

8:40 – 1193. Inelastic tunneling probe of bonds and chemical interactions. **W. Ho***

9:20 – 1194. Construction and manipulation of individual molecules: From reversible conductance transition to reversible single spin control. **H. Gao**

10:00 – 1195. Observation of Franck-Condon blockade in single molecules gated by local electric field. **A. Zhao**

10:20 Coffee break

10:35 – 1196. Recent progress in the study of single molecule chemistry at the nanometer length scale and picosecond time scale. **R.P. Van Duyn***

11:15 – 1197. Time-resolved tip-enhanced coherent anti-Stokes Raman scattering in an STM junction. **N. Tallarida**, J. Lee, L. Rios, K.T. Crampton, A. Zeytunyan, V.A. Apkarian

11:35 – 1198. Toward time-resolved single molecule chemistry: Probing plasmonic nanostructures with femtosecond light. **K.T. Crampton**, A. Zeytunyan, V.A. Apkarian*

Hawaii Convention Center
Halls I, II, III

Interplay between Theory and Experiment in Catalytic Research (#277)

Organized by: M. Ehara, C. Cramer, S. Dai, C. Jones, T. Ziegler, T. Tsukuda

Poster Session

10:00 – 12:00

1199. Experimental vs. computational ruthenium-xanthphos catalyzed olefin hydrogenation – can contemporary density functionals be used for in-silico-catalyst design prior to experimental art?. **M. Hölscher***, K. Rohrman, W. Leitner*

1200. Construction of QSAR model in catalytic asymmetric reactions by using L1-regularization method. **S. Yamaguchi***, T. Nishimura, H. Sato

1201. Density functional theory investigation of planar and cubane tetrametallic complexes of first-row transition metals for catalytic hydroxylation. **F. Spillebout***, O. Zelyak, S. Stoyanov, J. Stryker, A. Kovalenko

1202. Accurate thermochemistry by harmonic solvation model: Application to catalytic reactions in solution. **A. Ishikawa***, H. Nakai

1203. Tuning of barrier gaps between competing reactions. **C. Ehm***, P.H. Budzelaar, V. Busico

1204. Reactivity of Mo-Mo multiple bond and its application to catalytic reaction: Theoretical understanding. **Y. Chen, S. Sakai**

1205. Computational study on Cp*Ir complex-mediated 1-phenylethanol dehydrogenation and acetophenone hydrogenation with or without existence of acidic compounds. **E. Maeyama**, M. Sumimoto, K. Hori*

1206. Theoretical study of the nucleophilic substitution reaction via complex formation of propargyl alcohol derivatives and SnCl₂. **M. Nakamura***, S. Nanbu

1207. Reaction mechanism of fructose dehydration to 5-hydroxyl-methyl-furfural on external surface of H-ZSM-5 zeolite. **S. Namuangruk***

1208. Adsorption characteristics of thiophene on seven transition metal surfaces: A density functional study. **L. Wang*, L. Zhao*, J. Ji, C. Xu, J. Gao**

1209. Low-temperature reduction of N₂ with H₂ on palladium surfaces. **J. Murakami***, M. Futamata, K. Bando, Y. Shimo

1210. Chemical reactivity of metal-supported ceria thin films: A DFT+U study. **L. Szabova**, V. Matolin, Y. Tateyama, S. Fabris

1211. Theoretical studies on interaction between metal cluster and ceria: The role of ceria in CO adsorption. **R. Kindaichi***, H. Ushiyama, K. Yamashita

1212. Theoretical studies on the mechanism of alkali carbonate loaded on aluminosilicate catalysts for soot combustion. **T. Imamura***, H. Ushiyama, K. Yamashita

1213. Oxidation of silanes to silanols on Pd nanoparticles:H₂ desorption accelerated by surface oxygen atom. **T. Kamachi***, K. Shimizu, K. Igawa, K. Tomooka, K. Yoshizawa

1214. DFT study on reaction mechanisms for selective photocatalytic oxidation of benzyl alcohol on partially hydrated anatase (101) surfaces. **H. Kobayashi***, S. Higashimoto

1215. Reaction mechanism of ethylene epoxidation on a mesoporous metal-substituted silica heterogeneous catalyst: An experimental and theoretical investigation. **P.D. Patel***, W. Yan, A. Ramanathan, B. Subramaniam, B.B. Laird, W.H. Thompson

1216. Practicable measure and visualization of static electron correlation effects and its application for catalysts modeling. **A. Hansen***

1217. Mechanism of NO reduction on a di-nuclear metal complex. **K. Yoshizawa***, H. Tanaka, T. Suzuki, Y. Shiota, S. P.K., Y. Ankawa

1218. Understanding the formation process and selective nitrile hydrogenation performance of Ru nanocatalysts on K-Al₂O₃ by in-situ spectroscopy and theoretical calculation. **S. Muratsugu***, S. Kityakan, F. Wang, N. Ishiguro, O. Sekizawa, T. Uruga, T. Kamachi, K. Yoshizawa, M. Tada

1219. MoS₂ supported platinum single atom and its superior catalytic activity for low temperature CO oxidation: A density functional theory study. **H. Lin***, Y. Li*

1220. Immobilizing metal nanoparticles on single wall nanotubes. Effect of surface curvature. **A. Staykov***, T. Ishihara

1221. Computational study of the heterojunction effect in polymer-stabilized Au cluster. **K. Sakata***, K. Tada, A. Oguni, Y. Kondo, T. Saito, T. Kawakami, S. Yamanaka, M. Okumura

1222. DFT calculations for the investigation on the phenomena during preparation of Au cluster supported catalysts. **K. Tada***, H. Koga, K. Sakata, A. Oguni, Y. Kondo, T. Saito, T. Kawakami, S. Yamanaka, M. Okumura

1223. Synthesis of dendronized gold clusters with peptide-dendron-thiolates. **K. Ishibashi**, K. Isozaki, H.R. Takaya, M. Nakamura*

Hawaii Convention Center
312

Quantum Coherence in Energy Transfer: Electronic Energy Transfer in Molecular Systems (#297)

Organized by: J. Cao, P. Brumer, J. Wu

8:00 – 1224. Nature and role of coherence in photosynthetic light harvesting. **B. Whaley***

* Principle Author

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8:35 – 1225. Persistent electronic coherence despite rapid loss of electron-nuclear correlation. **A. Akimov**, O. Prezhdo
9:10 – 1226. Anomalous localization and optics of excitons in nanotubular molecular aggregates. **J. Knoester***
9:45 – 1227. A few lessons from non-adiabatic excited state dynamics simulations of large molecules. **S. Tretiak**
10:20 – 1228. New frontier in electronic structure: Establishing the connection between electronic correlation and decoherence. **I. Franco***
10:55 – 1229. Localized operator partitioning method for electronic energy transfer. **A. Izmaylov***
11:25 – 1230. Highly efficient energy transfer in FMO: Optimization and cluster-based dynamics. **J. Wu**

Hawaii Convention Center
306A

Science with Beams of Radioactive Isotopes (#340)

Organized by: S. Yennello, K. Starosta,
Y. Zhao, H. Haba
Presiding: H. Haba

8:00 – 1231. S_nRIT project at RIBF, RIKEN - exploring symmetry energy at supra-density. **T. Murakami**
8:30 – 1232. Dipole response of exotic nuclei and the nuclear symmetry energy. **T. Aumann**
9:00 – 1233. Learning from the continuum structure of light nuclei. **L.G. Sobotka***
9:30 Break
9:45 – 1234. Partial dynamical symmetries in nuclei. **R.F. Casten***, R. Cakirli,
A. Couture
10:05 – 1235. In-trap decay spectroscopy for electron capture branching ratios using TITAN at TRIUMF. **C. Andreoiu***
10:25 – 1236. Measured charge density difference between the isotones ²⁰⁶Pb – ²⁰⁵Tl. **S. Shlomo***
10:40 – 1237. Investigating the low-lying structure of ⁴⁶Ca from the β^- decay of ⁴⁶K. **J.L. Pore**
10:55 – 1238. Doppler shift lifetime measurements using the TIGRESS Integrated Plunger. **A. Chester**

Hawaii Convention Center
305B

Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344)

Organized by: D. Kilin, S. Kilina,
I. Burghardt, G. Scholes, U. Diebold,
A. Selloni, X. Gong, Q. Sun, R. Asahi,
K. Donnen
Presiding: V. Batista, S. Kilina

8:00 – 1239. Quantum dynamics of exciton migration and dissociation in functional organic polymer materials. **I. Burghardt***,
R. Binder, J. Wahl, H. Tamura
8:30 – 1240. Energy and charge transfer in polynuclear metal complexes. J. Tate,
s. Yamazaki, A. cadranel, P.S. Oviedo,
L.M. Baraldo, V. Kleiman
9:00 – 1241. Engineered semiconductor quantum dots for solar energy conversion. **V.I. Klironov***
9:30 Break
9:40 – 1242. Nonadiabatic molecular dynamics of singlet fission and charge separation. **A. Akimov***, O. Prezhdo
10:05 – 1243. Large-area quantum dot-based luminescent solar concentrators: General considerations and Monte Carlo ray tracing modeling. **K.A. Velizhanin***
10:30 – 1244. Photomobilities at nanostructured semiconductor surfaces from ab initio atomic modeling: A combined density matrix and energy band states treatment of excited electrons and holes at Si surfaces. **D.A. Micha***, R.H. Hembree,
T. Vazhappilly
11:00 – 1245. Technical and operational perspective on the DOE energy innovation hub in fuels from sunlight, the Joint Center for Artificial Photosynthesis. **N.S. Lewis***

11:30 Concluding remarks

Hawaii Convention Center
305A

Practical Strategies for Modeling Non-Covalent Interactions (#372)

Organized by: G. Beran, Y. Jung,
H. Nakai, J. Schmidt
Presiding: J. Schmidt

8:00 – 1246. Effective fragment potential method for biological systems. **L. Slipchenko**

8:30 – 1247. Energy decomposition analysis of intermolecular interactions from block-localized density functional theory. **J. Gao**

9:00 – 1248. Accurate, ab-initio-quality PES for H₂ adsorbed to MOF-5. **J. D'Arcy***, M. Jordan, T.J. Frankcombe, M. Collins

9:20 – 1249. Ab initio many-body potentials for chemically accurate simulations from the gas to the condensed phase. **F. Paesani**

9:50 Break

10:00 – 1250. Insight into structure and transport of battery electrolyte from molecular simulation. **O. Borodin***, M. Olguin, K. Xu, L. Suo, C. Wang, W. Henderson

10:30 – 1251. High performance polarizable molecular dynamics: Large scale modeling of noncovalent interactions. **J. Piquemal***

11:00 – 1252. Visualizing cooperativity: Non-additive contributions to the deformation density. **C. Mück-Lichtenfeld***

11:20 – 1253. Fixed diabatic atomic charge formalism: An efficient route for simulating dynamics with electronic excitations. **Y. Rhee**

11:50 Closing Remarks

Hawaii Convention Center
304B

Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403)

Organized by: A. Amirfazli, Y. Zuo, J. Li
Presiding: K. Ariga, J. Huang, T. Liedl,
D. Pang

8:00 – 1254. Hand-operating nanotechnology: Manual handling of molecular machines at interfaces. **K. Ariga**

8:30 – 1255. Self-assembly of DNA origami arrays on lipid membranes. **T. Liedl***

8:55 – 1256. Peptides-modulated self-assembly of photoactive dyes toward complex functional systems. **X. Yan***

9:20 – 1257. On the formation of lipid nanoscale structures at interfaces beyond planar bilayers. A. Dabkowska, C. Niran, G. Piret, H. Persson, H. Wacklin, H. Linke, C. Prinz, T. Nylander*

9:45 – 1258. Molecular-scale mechanism of protein adsorption resistance of oligo(ethylene glycol) terminated-SAMs investigated by frequency modulation AFM in liquid. **N. Inada**, H. Asakawa, K. Miyazawa, T. Fukuma*

10:05 Coffee Break

10:15 – 1259. Controllable live-cell synthesis of fluorescent semiconductor quantum dots: How to have cells do what they cannot do? **D. Pang***, R. Cui, Y. Li, H. Liu, Z. Xie, Z. Zhang, B. Hu

10:40 – 1260. Bioinspired controllable liquid transfer by topological asymmetric fibers. **H. Liu***, L. Jiang

11:00 – 1261. Underwater wettability of bioinspired adhesive surfaces. **B. Soltannia, D. Sameoto , P.R. Waghamare***

11:20 – 1262. Numerical simulation and experimental study on the mass transport in biogranules with implication to their deformable feature. **W. SUN***, X. Li

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable,
K. Liu, J. Lane, Y. Kajii, X. You
Presiding: S. Kable

8:00 – 1263. Directly measuring the kinetics of key intermediate species in hydrocarbon oxidation. **C.A. Taatjes***

8:30 – 1264. The biosphere is CO₂L? The role of reactive intermediates in offsetting climate change. D. Shallcross, **A.H. Khan**

9:00 – 1265. Microwave perspective on the chemistry of reactive oxygen molecules. **M.C. McCarthy***

9:30 – 1266. Directly detecting QOOH radicals: Key intermediates in combustion and atmospheric chemistry. **D. Osborn**

10:00 – 1267. Atmospheric autoxidation via fast hydrogen shift reactions. **H.G. Kjaergaard**

10:30 – 1268. Underemployed and looking for action: The plight of unpaired electrons in reactive intermediates and other elusive species. **A. Sanov***

11:00 – 1269. Role of polycyclic aromatic hydrocarbons with a multiradical character in soot formation. **X. You***

11:30 – 1270. Toward high-level theoretical studies of large biodiesel molecules: An ONIOM [QCISD(T)/CBS-DFT] study of reactions of unsaturated methyl esters with hydrogen radical. L. Zhang, **P. Zhang***

Hawaii Convention Center
307AB

Structure and Spectroscopy of Linear Polyenes: Finite and Infinite (#456)

Organized by: B. Hudson, N. Hush,
T. Kobayashi, Y. Weng, J. Paldus,
R. Christensen
Presiding: T. Kobayashi

8:00 – 1271. Butadiene, the simplest polyene? Not by a long shot. **R.J. Cave***, S. Rabidoux, J. Stanton

8:30 – 1272. Defining and (at least partly) meeting the challenges of developing electronic structure methods suitable for describing polyenes. **M. Head-Gordon**

9:00 – 1273. Bootstrap embedding. **M. Welborn**, T. Tsuchimochi, T. Van Voorhis

9:30 – 1274. Non collinear Hartree-Fock solutions of fullerenes and other carbon systems. **G. Scuseria***, C. Jimenez-Hoyos

10:00 – 1275. Electronic structure of trans-polyenes from two electron functions. **K. Boguslawski***, P. Tecmer, P. Ayers

10:30 – 1276. The many particle expansion: A systematic method for removing self-interaction from DFT. **T. Van Voorhis**, T. Zhu, H. van Aggelen

11:00 – 1277. Large scale modelling of strong electron correlation effects in extended systems from geminals. **P. Tecmer***, K. Boguslawski, P. Ayers

11:30 – 1278. Not just linear polyenes: The intriguing case of squaraine dyes. **C. Sisca***, S. Sanyal, F. Avila, J. Cerez, F. Santoro, A. Painelli

Hawaii Convention Center
Halls I, II, III

Physical, Theoretical & Computational General Posters

Presiding: M. Waterland, K. Yamanouchi
10:00 – 12:00

Data Base Development

1279. InChI – recent developments in the worldwide IUPAC chemical structure identifier standard. **S. Heller***

Gas Phases (Experimental)

1280. Characterizing the electronic states of gold monosulfide, AuS. **T.D. Varberg***, B.W. Pearlman, I.A. Wyse, D.L. Kokkin, R. Zhang, T.C. Steinle

1281. A step closer to understanding acid solvation: Dissociation dynamics of mixed HCl and H₂O clusters. **K. Zuraski**, D. Kwasniewski, A.K. Samanta, H. Reisler*

1282. Electronic state separation of NH_n⁺ (*n*=1–3) in ion mobility measurements. **K. Mori**, T. Yamazaki, H. MAKI, A. NINOMIYA, H. Tanuma*

1283. Direct observation of relaxation of nitric oxide Rydberg states to a strongly coupled plasma. **H. Sadeghi Esfahani*** Liquids (Experimental)

1284. Photoreduction yields of Sm³⁺ and Yb³⁺. **M. Kusaba***

1285. Excess enthalpies of propylamine and alcohol isomers. **H. Hayashi**, T. Kamiyama, K. Takayoshi

1286. Hydration behavior of substances bearing tertiary amino group. **N. Sagawa**, T. Shikata

1287. Rebinding dynamics of NO to microperoxidase-8 probed by femtosecond IR spectroscopy. T. Lee, S. Park, H. Kim, M. Lim*

1288. Ultrafast terahertz Kerr effect spectroscopy of aromatic liquids. **I.A. Finnigan***, M. Allodi, G. Blake

1289. Experimental and computational thermodynamic characterization of naphthoxazoles derivatives in beta- and gamma-cyclodextrins. **S. Valdebenito***, A. Zanocco, G. Zapata-Torres

1290. Study of electronic states of aqueous solutions of sodium halides by using temperature dependence attenuated total reflectance spectroscopy in the far ultraviolet region. **Y. Nishikawa**, Y. Morisawa, A. Ikebata

1291. High pressure solubility and partial molar volume of L-tyrosine in water at 298.2 K. **S. Sawamura***, E. Atsuda

1292. Raman spectroscopic and density functional calculations investigations on water molecules in tetrahydronafuran clathrate hydrate. **M. Kato***, S. Matsumoto, A. Takashima, Y. Fujii, Y. Takasu, I. Nishio

1293. Considerations on the hydrogen bond formation and proton transfer in methylpyridinium-alcohol system by spectroscopy and theoretical method. **N. Iwasaki**, M. NIWA, S. Tanaka, T. SUZUKI

Surfaces and Clusters

1294. Photocatalytic hydrogen formation by Pt/Au/WO₃ under visible light. **A. Tanaka**, H. Kominami

1295. Comparison of self-assembled structures of the unnatural amino acid vs. naphthalene on Au(111). **S. Yang**, H. Lee

1296. Step sensitive mechanism of CO₂ hydrogenation on copper surface of Cu/ZnO/Al₂O₃ catalyst. **Y. Kim**, H. Lee

1297. Preparation of titania thin films in the adsorbed water layer formed at the solid/organic solvent interface. **T. Kenmotsu***, H. Endo, K. Torigoe, K. Sakai, M. Abe, H. Sakai

Soft Matter (Experimental)

1298. Antiparallel dimer formation of 4-cyano-4'-alkylbiphenyls in isotropic cyclohexane solution. **S. Takabatake**, T. Shikata

1299. Hierarchical self-organization dynamics of millimeter-long helical assembly composed of oleic acid. **Y. Kageyama***, T. Ikegami, S. Takeda

* Principle Author

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onlineprogram

- 1300.** Effect of industrial waste on chemical resistance and water absorption of bamboo fibre reinforced epoxy composites. **A. Gupta***
- 1301.** Generation dependent ultrafast charge transfer dynamics in pyrene-viologen dendrons. **Z. Gong***, J. Bao*, T. Iyoda, T. Kawachi, P. Piotrowiak*
- 1302.** Polarity effect of exterior chains on self-assembled structure and aggregation mechanism of tetraphenylethene derivatives in THF/water mixture. **S. Cho**
- Solids (Experimental)**
- 1303.** Dehydration process of crystal of metal salt hydrate. **S. Yoshida**, T. Miyaji, T. Kamiyama, K. Takayoshi
- 1304.** Structural change of vapor deposited H_2O-CO_2 amorphous ice with warming. **R. Netus**, T. Ikeda-Fukazawa
- 1305.** Evaluation of the magnetic properties of cuprate molecular spin ladders. **S. Nishihara***, X. Zhang, Y. Nakano, K. Maryunina, K. Inoue*
- 1306.** Electrochemical studies of copper (II) ion using voltammetric method and digital simulation at HMDE. **A. ALOWAIS***
- Development of DFT**
- 1307.** Application of the space-pseudo-time method to Kohn-Sham and orbital-free density functional theory. **D. Gebremedhin, C. Weatherford**
- 1308.** Novel correction on DFT noncovalent interactions based on S22, S66, and X40 benchmark databases. **L. Hu***, L. Li, H. Li
- 1309.** Applications of machine learning on quantum chemical databases. **A.R. Cameron***, J. Pearson
- 1310.** Probing interelectronic interactions with the localized pair model. **A.J. Proud***, D.E. Mackenzie, J. Pearson
- Theoretical Calculations**
- 1311.** Correction system for efficient prediction of molecular physicochemical properties based on machine learning. **H. Li***, L. Hu, T. Gao, H. Li, C. Fang, J. Huang
- 1312.** Potential energy curves for excited states of selected alkali metal diatomics with multireference coupled cluster method. **M.A. Musial***
- 1313.** Search for variation of fundamental constants: Strong enhancements in χ^2_{II} cations selected diatomics. **L.F. Pasteka***, A. Borschkevsky, P. Schwerdtfeger, V.V. Flambaum
- 1314.** Application of relativistic prolapse-free basis sets in obtaining of fundamental properties of the homonuclear barium and radium dimers. **T.Q. Teodoro**, R.L. Haiduke, U. Dammalapati, S. Knoop, L. Visscher
- 1315.** Applications of time-dependent and time-independent density functional theory to Rydberg transitions. **I. Seidu**, M. Kryukov, T. Ziegler*
- 1316.** Novel method for determining the mean-field directly from the single particle matter density: Application to the measured charge density difference between the isotopes ^{206}Pb , ^{205}Tl . **S. Shlomo***
- 1317.** Theoretical study for methane activation on zinc modified ZSM-5 zeolite system. **Y. Park***, Y. Kim
- 1318.** Theoretical study of acetylation of ethylamine catalyzed by M^{2+} ions. **S. Caglioti***, G. Servetti
- 1319.** New method for designing effective fields that mimic catalytic fields based on linear response function of bond order. **S. Yamamoto***, Y. Mitsuta, T. Kawakami, M. Okumura, . Nakamura
- Chemical Reactions (Theory)**
- 1320.** Mechanistic study of methanol oxidation by Ru^{IV} -oxo complexes. **Y. Shiota***, T. Kojima, K. Yoshizawa
- 1321.** Automated mapping and computation of the complete rearrangement networks of substituted bulyvalene. **L.F. Pasteka***, T. Fallon, P. Schwerdtfeger
- 1322.** Theoretical studies of hydroformylation of butadiene. **C.H. Mendis***, W.H. Thompson, J.A. Tunje, T. Maji
- 1323.** Using the global reaction route mapping strategy to explore methylation effects on carbocation precursors to terpenes. **B. Hudson***, R. Ramozzi, C. Sameera, K. Morokuma, D.J. Tantillo
- 1324.** Efficient algorithm of finding chemical reaction pathways: Stochastic and deterministic. **Y. Kim***, S. Choi, J. Kim, W. Kim*
- Solutions (Theory and Computational)**
- 1325.** Understanding the comparative molecular field analysis (CoMFA) within the framework of molecular quantum similarity and chemical reactivity descriptors using density function theory. **A. Morales-Bayuelo**
- 1326.** Diffusion-influenced reactions facilitated by dimension reduction. **H. Kim**
- 1327.** Application limitations of analytical solution to determine intraparticle diffusivity from concentration decay curve. **Y. Nakayama***, N. Sonetaka, Y. Seida, E. Furuya
- 1328.** Sensitivity of the linear responses function of the bond orders for the conformation. **Y. Mitsuta***, S. Yamanaka, T. Kawakami, T. Saito, M. Okumura
- 1329.** First-principles calculation of NMR shielding in paramagnetic molecules including magnetic couplings. **S. Rouf***, J. Mareš, J. Vaara
- 1330.** Prediction of biodegradability and toxicity of aromatics in water using QSAR modeling. **J. Dermadi, D. Juretic, M. Novak Stankov, H. Kusic, S. Ukić, T. Bolanca, A. Loncaric Bozic***
- 1331.** Density functional theory benchmark for the structure and reactivity of frustrated Lewis pairs. **Q. Almas***, J. Pearson
- 1332.** Method optimization for UV/visible spectrum calculations of indigoid dyes and complexes. **S.W. MacLean***, R. Hicks
- 1333.** Solvent effects on azobenzene derivative photodynamics with spin-flip time-dependent density functional theory and effective fragment potential methods. **K. Keiper**, Y. Harabuchi, M. Gordon
- 1334.** New concept for high power target and new concept energy system. **L. Yang***
- Solids and Interfaces (Theory)**
- 1335.** Adsorption and diffusion of proton on amorphous ice. **M. Aoki***, T. Ikeda-Fukazawa
- 1336.** Surface structure of amorphous ice. **Y. Kumagai**, T. Ikeda-Fukazawa
- 1337.** Studying the phase transition of multi-ferroics thin film by Landau theory. **A.M. Alrub**
- 1338.** Na doped $\text{Sr}_2\text{CrOsO}_6$, a novel half metal predicted by first principles. **Z. Wu***
- 1339.** Magnetic and electronic structure of Mn_2CuSi and Mn_2ZnSi half-metallic inverse Heusler alloy. I.H. Bhat*, D.C. Gupta
- 1340.** Studies on optimized operational conditions for experimental determination of mass transfer properties with the circulating-type fixed-bed adsorber method. **K. Teshima***, E. Furuya, J. Fujiki, T. Kawakita, K. Watanabe
- 1341.** Time-dependent electron wave packet dynamics of transient current in 1D array of quantum dots. **T. Sako***
- 1342.** Thermodynamic scaling of dynamic properties in liquid crystalline phase. **K. Sato***
- 1343.** Theoretical approach to the carbon deposition avoidance on the surfaces of $\text{BaTiO}_3(001)$. **D.S. Rivera Rocabado***, T. Ishimoto, M. Koyama
- 1344.** Molecular study on adhesion phenomena. **T. Semoto***, K. Yoshizawa
- 1345.** Influence of solution-phase and mesoporous environments on excited state lifetime in 9-mesityl-10-methylcaridinium. **N. Garcia**, T. Kowalczyk*
- 1346.** Study of the interfacial array behavior of surfactant at very low concentration by second harmonic generation and molecular simulation. **D. Li***, H. Pan, Y. Li
- 1347.** CO oxidation reactivity on the CO-covered Pt nanoparticle. **D. Kim***, J. Lee, J. Park, S. Lee, M. Jeong, Y. Jo
- 1348.** Alloy catalyst configuration and adsorbate distribution revealed via first principles based Monte Carlo simulations. **T. Tan***, L. Wang, D. Johnson, J. Zhang
- 1349.** Density functional theory study of transition metal and metal alloy catalysts in energy production. X. Wu, Y. Lu, S. Tsang, **X. Gong Polymers (Theory)**
- 1350.** Molecular simulations of single-walled carbon nanotubes grafted with polymers. **H. Lee***
- 1351.** Density functional theoretical study on dialkoxyphenylene-benzothiadiazole-containing photovoltaic polymers. **S. Hwang**, H. Woo
- 1352.** Density functional theoretical and time-dependent density functional theoretical study on thiophene-benzothiadiazole-based polymers. **Y. Cho**, S. Hwang, H. Woo
- 1353.** Density functional theoretical study on benzodithiophene-thiophene-based photovoltaic polymers. **Y. Lee**, S. Hwang, H. Woo
- Biophysics (Theory)**
- 1354.** Rational design and synthesis of selective blockers of the K_2P channel TASK-3. **B.a. Arevalo***, L. Zúñiga, M. Gutierrez, W. Gonzalez
- 1355.** Third-generation density functional calculation program: ProteinDF. **T. Hirano**, F. Sato
- 1356.** Study of protein aggregation as a process of cataract formation. **V. Prytkova**, M. Heyden, D. Tobias
- 1357.** Evaluation of physical properties using thermodynamic quantities of hydration. **M. Fujisawa***, h. Ikeda, M. Okanami, K. Takayoshi
- 1358.** Evaluation of structural differences between estrogen receptor α and β using the ligand binding site search program HBOP/HBSITE. **K. Fujii***, S. Fukuyoshi, N. Yamaotsu, S. Hiroto, A. Oda
- 1359.** Source of the drug resistance toward the mutation of influenza neuraminidases: MD and 3D-RISM studies. **J. Phanich, T. Rungratmongkol***, S. Hannongbua
- 1360.** Development of bioinspired catalysts for efficient peptide hydrolysis. **R. Prabhakar***
- 1361.** Revealing monoamine oxidase B catalysis mechanisms using quantum chemical cluster approach. **G. Zapata-Torres***, A. Ferro, C. Celis-Barros
- 1362.** In silico identification of small molecules that modulate the aminoglycoside-sensing riboswitch. **S. Park***, G. Lee, H. Park*
- 1363.** Structural prediction of wild-type and mutant CYP1A2 complexed with 7-ethoxyresorufin using docking and molecular dynamics simulations. **Y. Watanabe***, S. Fukuyoshi, M. Hiratsuka, N. Yamaotsu, S. Hiroto, A. Oda
- 1364.** Stability and dynamics of beta-sheet aggregates of polyalanine peptides. **J. Kim***
- 1365.** Theoretical study on $[\text{Ru}(\text{bpy})_2\text{dpdz}]^{2+}$ at well-matched and mismatched sites for binding structures and interactions with the neighboring DNA. **M. Otsuka**, K. Takano
- Friday Afternoon**
- Hawaii Convention Center 301B
- Synergistic Relationships between Computational Chemistry and Experiment (#9)**
- Organized by:** S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: N.M. Cann, Y. Wu
- 13:00 Break**
- 13:10 – 1366.** Conical intersections with density-functional theory? **A. Becke***
- 13:30 – 1367.** Dispersion-corrected DFT for molecular crystals and polymorphism. **E.R. Johnson***, S.R. Whittleton, A. Otero-de-la-Roza
- 13:50 – 1368.** Density functional model for nondynamic and strong correlation. **J. Kong***, E. Proynov
- 14:10 – 1369.** Steady-state density functional theory and its applications. **C. Zhang**
- 14:30 – 1370.** New and improved energy decomposition analysis: Well-defined physical contributions to intermolecular interactions from density functional theory calculations? **M. Head-Gordon**
- 14:50 – 1371.** Density functional theory for accurate potential energy surfaces. **W. Kim***
- 15:10 Break**
- 15:20 – 1372.** Some new ways to do excited states for large molecules. **R.J. Bartlett***, J. Byrd, D. Bokan, V. Rishi
- 15:40 – 1373.** Electronic communication across noncovalent interactions on vinyl silyl bridged bisferrocenyl compounds. **O. Mo***, M. Montero-Campillo, S. Bruña, I. Cuadrado
- 16:00 – 1374.** Fresh perspective on the spectroelectrochemistry of ferrocene derivatives. **J.R. Lane***
- 16:20 – 1375.** Electronic spectroscopy and photochemistry: Solvent effects and dynamics. **M.S. Gordon***
- 16:40 – 1376.** Single-determinant models of excited states. **G. Barca, A. Gilbert, P. Gill***
- Hawaii Convention Center 306A
- Coarse Grained Modeling and its Integration with Experiments (#30)**
- Organized by:** R. Faller, D. Huang, M. Karttunen
Presiding: D.M. Huang
- 13:00 – 1377.** Systematic and simulation-free coarse graining of polymer melts. **Q. Wang***
- 13:50 – 1378.** Systematic multiscale modeling for photovoltaic applications. **T.F. Harrelson, A. Moule, R. Faller***
- 14:20 – 1379.** Polymers in inorganic scale control: Molecular dynamics study of edge-active polymers. **E.J. Smith***, C. Fellows
- 14:50 – 1380.** In-depth exploration of the self-assembling mechanisms of a designed lytic peptide by molecular dynamic simulation. **S. Luo***, F. Sun
- 15:20 – 1381.** Common physical framework explains phase behavior and dynamics of atomic, molecular, and polymeric network-formers. **S. Whitelam**
- Hawaii Convention Center 308A
- Modeling and Analyzing Exciton and Charge Dynamics in Molecules and Clusters (#44)**
- Organized by:** S. Tretiak, G. Chen, Y. Tanimura
Presiding: V.Y. Chernyak
- 13:00 Opening Remarks**
- 13:05 – 1382.** Photoinduced dynamics in nanoparticles: Time-domain ab initio studies. **O. Prezhdo**
- 13:35 – 1383.** Efficient semiclassical method for modeling non-adiabatic dynamics in multiaatomic molecules. **D. Mozyrsky***
- 14:05 – 1384.** Manipulation of light-matter interaction at the nanoscale. **Y. Luo**
- 14:35 Break**
- 14:50 – 1385.** Optical properties of graphene derivatives. **H. Su***, X. Zhu

* Principle Author

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15:20 – 1386. Energy-specific excited state electronic structure methods for modeling high-energy exciton and charge dynamics. **X. Li***, B. Peng, P.J. Lestrange
15:50 – 1387. Role of surface defects and ligands in energy transfer and nonradiative relaxation in quantum dots. **S. Killina***
16:20 – 1388. Molecular-level details of morphology-dependent exciton migration in poly(3-hexylthiophene) nanostructures. **P.C. Tapping***, S.N. Claffon, K.N. Schwarz, T.W. Kee, D.M. Huang

Hawaii Convention Center
313B

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: A. Bertram, X. YANG
13:00 – 1389. On the heterogeneous uptake of ClO_2 on organic aerosol. **H.D. Osthoff***, J. Liglio, S.G. Moussa
13:30 – 1390. Laboratory and field studies of heterogeneous uptake of HO_2 radicals to aerosols and clouds. **D. Heard***, L. Whalley, D. Moon, C. Kidd, P. Lakey, G. Cousins, P. Seakins, I. George, M. Baeza-Romero, D. Stone, D. van Pinxteren, A. Tilgner, H. Herrmann, M. Evans, T. Berkemeier, M. Shiraiwa, S. Mertes, M. Ammann, J. Dommen
13:50 – 1391. Impacts of mixed aerosols on heterogeneous reactions of atmospheric particles. **S. Tong**, F. Tan, M. Ge
14:10 – 1392. Effects of temperature, pH, and ionic strength on the Henry's law constant of atmospheric amines. **Y. Liu**
14:30 – 1393. Heterogeneous reactions of atmospheric oxidizing gases with soot. **H. He***

15:00 Break
15:10 – 1394. Microspectroscopic examination of atmospheric ice nucleating particles. **D.A. Knopf***, P.A. Alpert, D. Bothe, J.C. Charnawskas, W. Kilthau, B. Wang, R. O'Brien, R. Moffet, M.K. Gilles, A. Laskin, J.Y. Aller
15:40 – 1395. Dynamic ice nucleation studies on laboratory-generated and field-collected atmospheric particles using a microscopic imaging platform. **B. Wang***, D.A. Knopf, M.K. Gilles, A. Laskin
15:55 – 1396. Climatology of ice nucleating particles at the high altitude station Jungfraujoch. **Z.A. Kanji***, Y. Boose, L. Lacher, U. Lohmann
16:10 – 1397. On the relationship between acidic aerosols and types of ice clouds over the North Slope of Alaska. **E. Girard***
16:25 – 1398. Observations of aerosol particles and low cloud in the summertime Arctic. **R. Leaitch***, J. Burkart, M. Willis, F. Koellner, J. Schneider, H. Bozem, P. Hoor, A. Herber, J.P. Abbott

Hawaii Convention Center
308B

Advances in Quantum Monte Carlo (#80)

Organized by: S. Tanaka, L. Mitas, P. Roy
Presiding: L. Mitas
13:00 – 1399. Recent progress in FCIQMC. **A. Alavi**
13:35 – 1400. Optimization of many-body wavefunctions by minimizing the fixed-node projector Monte Carlo energy. **C.J. Umrigar**, J. Toulouse, M. Otten, R. Assaraf
14:10 – 1401. Using perturbatively selected CI expansions in fixed-node diffusion Monte Carlo. **M. Caffarel***, E. GINER, T. APPLENCOURT, A. Scemama
14:45 Break
14:55 – 1402. Tensor network quantum Monte Carlo. **G.K. Chan**, B. Verstichel
15:30 – 1403. Model space quantum Monte Carlo method for degenerate and quasi-degenerate electronic states. **S. Ten-no**
16:05 – 1404. Dissection of a covalent bond through quantum entanglement. **N. Tubman**

Hawaii Convention Center
305B

Recent Advances in Dynamics of Confined Liquids (#123)

Organized by: A. Luzar, G. Patey, M. Kinoshita
Presiding: C. Neto
13:00 Opening Remarks - Luzar
13:05 – 1405. Correlated nonequilibrium response in nanoconfined systems. **D.T. Limmer***

13:35 – 1406. Molecular theory of hydrodynamic boundary conditions in nanofluidics. **A.E. Kobryn**, A. Kovalenko
14:05 – 1407. Viscosity of aqueous electrolyte solutions: The dynamic point of view for hydrophobicity and hydrophilicity. **J. Dufreche***, J. Molina, B. Siboulet, M. Duval, P. Turq, B. Bagchi
14:35 – 1408. Effect of electric field on water molecules confined in carbon nanotubes. **.. Winarto***, D. Takaiwa, E. Yamamoto, K. Yasuoka

15:05 break
15:20 – 1409. Static and dynamic boundary conditions for confined ionic liquids. **J. Ralston***, M. Krasowska
15:50 – 1410. Ordered nonwetting water, water-surface composition structure, evaporation, and heat transfer on the surfaces studied using molecular dynamics simulations. **H. Fang***, C. Wang, P. Guo, y. Tu, R. Wan, J. Chen
16:20 – 1411. Microfluidics in micropillar arrays. G. Holzner, F.H. Kriel, **C. Priest***

Hawaii Convention Center
304A

Self-organization in Chemistry (#165)

Organized by: S. Nakata, J. Pojman, O. Steinbock, Q. Gao, J. Wang, T. Yamaguchi, R. Yoshida, S. Nakabayashi
Presiding: T. Aramemiya, A.F. Taylor, T. Yamaguchi

13:00 – 1412. Spontaneous rotation of colloidal fluids in electroconvective flows under gravity. **M. Sano***

13:15 – 1413. Hierarchical self-organization: From nanorods to biomorphs and macroscopic tubes. **O. Steinbock***, E. Nakouzi, B. Batista

13:45 – 1414. Wave-particle duality in dissipative systems. **Y. Nishiura***

14:15 – 1415. Dynamics of chemical self-replication in artificial peptide networks. **E. Peacock-Lopez**

14:35 – 1416. Self-organized ordering in skin tissue. **S.K. Schnyder***, R. Yamamoto

14:50 coffee break

15:05 – 1417. Non equilibrium structured nanomolecular assemblies. **L. Cronin***

15:30 – 1418. Motion of a Belousov-Zhabotinsky reaction droplet coupled with pattern formation. **H. Kitahata**

15:50 – 1419. Mechanism of the generation of stochastic nature of the Soai system. **K. Asakura***, S. Iamurra, H. Mashimo, T. Banno, K. Tako

16:10 – 1420. Synchronization in populations of chemical oscillators: Phase clusters and chimeras. **K. Showalter***, M. Tinsley, S. Nkomo, A. Taylor, F. Wang

16:40 Discussion

16:55 Closing Remarks

Hawaii Convention Center
313C

Challenges in Plasmonic Photochemistry (#176)

Organized by: H. Misawa, P. Kamat, H. Sun, S. Gwo
Presiding: S. Gwo, T. Teranishi
13:00 Opening Remarks
13:05 – 1421. Surface-plasmon enhanced terahertz spectroscopy using gold nanostructured terahertz antennae. **K. Ueno**, S. Nozawa, H. Misawa

13:25 – 1422. Plasmon-based hot carrier photocatalysis. **N. Halas***
13:55 – 1423. Plasmon-enhanced chemistry: Theoretical studies. **G.C. Schatz**

14:35 – 1424. Large-scale hot spot engineering for quantitative single-molecule detection using SERS. H. Chen, M. Lin, C. Wang, Y. Chang, **S. Gwo***
15:05 – 1425. Single nanoparticle SERS studies of plasmonic photochemistry. **R.P. Van Duyn***

15:35 – 1426. Visible-to-NIR plasmonics in inorganic nanodisks. **T. Teranishi***
16:05 – 1427. Local optical activity and chirality of metal nanostructures. **H. Okamoto***, S. Hashiyada, T. Narushima, Y. Nishiyama

16:25 – 1428. Super-resolution and defocused microscopy on single molecules coupled with gold nanorod optical antennas. **J. Hofkens***, L. Su, H. Yuan, H. Ujii
Hawaii Convention Center
310 Theatre

Challenges and Opportunities for Exascale Computational Chemistry (#184)

Organized by: J. Rice, W. Swope, A. Rendell, Y. Okamoto
Presiding: W. Swope

13:00 Opening Remarks
13:05 – 1429. Algorithmic and software techniques for scaling quantum chemistry on massively parallel computers. **J.R. Hammond***

13:30 – 1430. Center for accelerated application readiness: Early experiences in preparing applications for the summit architecture. **T. Straatsma***

13:55 – 1431. Quantum chemistry on low-powered processors. **A.P. Rendell**, G. Mitra, K. Keipert, S.S. Leang, M.S. Gordon

14:20 – 1432. Hardware trends and the challenges for computational chemistry. **B. Austin***

14:45 Break

15:00 – 1433. Emerging computer architectures and their implications for computational chemistry. **R. Dror**

15:25 – 1434. Parallel computing with NTChem software for petascale supercomputing and toward exascale supercomputing. **M. Katouda***, T. Nakajima

15:45 – 1435. QuantumChemistry500 ranking: A benchmark suite for quantum chemical program packages and supercomputers. **M. Nakata***, K. Ishimura, T. Hirano, J.R. Hammond

16:05 – 1436. Enabling energy-efficient exascale computing on heterogeneous architectures with ARM. **K. Keipert**, S.S. Leang, M. Gordon, G. Mitra, A.P. Rendell

Hawaii Convention Center
306B

Metal Ions and Protein Functions: Theoretical Models and Applications (#202)

Organized by: Q. Cui, M. Meuwly, T. Allen, Y. Gao
Presiding: T.W. Allen

13:00 – 1437. Conduction and block of sodium channels by metal and organic cations: Computational and experimental viewpoints. **R.J. French***, R.K. Finol-Urdaneta, Y. Wang, S. Huang, K. Jia, S. Noskov

13:40 – 1438. Understanding sodium selective conduction using the bacterial Na^+ - Ab channel. **C. Boiteux, E. Flood, I. Vorob'ev, T.W. Allen**

14:20 – 1439. Hydration mimicry: A strategy for ion permeation through channel proteins? **M. Chaudhari, J. Vanegas, S. Rempe**

15:00 Break

15:00 – 1440. Role of electronic polarization effects in mechanisms of cation recognition by metalloproteins. **V. Ngo, M. Chagas Da Silva, H. Li, M. Kubillus, D. Salahub, Q. Cui, B. Roux, S. Noskov**

15:40 – 1441. Computational studies of ions solvation with ring polymer molecular dynamics. **I. dang***
16:20 – 1442. Structure and dynamics in ion solvation—from clusters to solutions. **Y. Gao**

Hawaii Convention Center
304B

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Eikerling, G. Jerkiewicz, S. Mitsushima, A. Gewirth
Presiding: B.D. Gates, A. Gewirth

13:00 Introductory remarks
13:10 – 1443. Sunlight-driven hydrogen formation by membrane-supported photoelectrochemical water splitting. **N.S. Lewis***

13:40 – 1444. Surface plasmon assisted photo-electrochemistry on microelectrodes. **W. Wang, Y.F. Huang, H. Guo, D. Zhan, D. Wu, B. Ren, Z. Tian**

14:10 – 1445. Catalytic activity and durability of $\text{Li}_{1-x}\text{O}_2/\text{Ni}$ anode for alkaline water electrolysis. **S. Mitsushima***, S. Fujita, Y. Kohno, I. Nagashima, Y. Sunada, Y. Nishiki, A. Manabe, K. Matsuzawa
14:30 – 1446. Redox catalysis and charge storage for indirect water electrolysis. **H.H. Girault***

15:00 Break

15:20 – 1447. Structure and reactivity in efficient electrocatalysis and photoelectrocatalysis. **P.J. Kulesza***

15:50 – 1448. Electrochemical and photoelectrochemical biomass valorization. **K. Choi**

16:10 – 1449. Study of surface reactivity of Li-ion positive electrode materials in organic carbonate electrolytes. **R. Kosteck***, A. Jerry

16:40 – 1450. On the mechanism of photocatalytic $\text{Ag}^{(II)}$ ion reduction under magnetic field. **H. OKUMURA***, S. Endo, E. YAMASUE, K.N. Ishihara

Hawaii Convention Center
312

Quantum Coherence in Energy Transfer: Coherence in Light-harvesting Energy Transfer (#297)

Organized by: J. Cao, P. Brumer, J. Wu

13:00 – 1451. Fano coherences in the molecular dynamics induced by incoherent light. **P. Brumer***, T. Ischerbul

13:35 – 1452. Quantum coherence in light-harvesting energy transfer. **J. Cao***

14:10 – 1453. Coherent transport enhancements in incoherent light harvesting. **I. Kassal**

14:45 – 1454. Water-soluble chlorophyll-binding protein (WSCP): An interesting system for the development of theory and modeling. **T. Renger**, T. Dinh, D. Lindorfer, F. Mühl, H. Lokstein, J. Adolphs, M. Berrer, M. Schmidt am Busch

15:20 – 1455. Chlorosome of green sulfur bacteria: Energy transfer dynamics and coherence. **A. Aspuru-Guzik**

* Principle Author

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15:55 – 1456. Classical multichromophoric resonance energy transfer. S. Duque, P. Brumer, **L. Pachon***

16:30 – 1457. Excitation energy transfer in photosynthetic and artificial light-harvesting systems: A coherent modified Red-field approach. **Y. Cheng**

Hawaii Convention Center
301A

Dynamical Intermolecular Interactions for Biological Functions (#307)

Organized by: D. Zhong, M. Terazima, Q. Lu

13:00 – 1458. Light-sensitive molecules for time-resolved crystallography and optogenetics. **K. Moffat***

13:35 – 1459. Novel photodynamics in photochrome and cyanobacteriochrome photosensory proteins. **D.S. Larsen***

14:05 – 1460. Probing protein structural dynamics with pump-probe X-ray lidography and crystallography. **H. Ihée***

14:35 – 1461. Analysis of gallstone component with Fourier transform infrared spectroscopy. **H. Mizumoto*, L. Li**

14:55 Break

15:10 – 1462. Time-resolved detection of inter-protein interaction during protein reaction. **M. Terazima***

15:40 – 1463. Secondary structure and intermolecular interaction of biomolecules at the interface investigated by sum frequency generation vibrational spectroscopy. **S. Ye, K. Lin, Y. Luo***

16:10 – 1464. Mechanism of amyloid formation of human calcitonin. **M. Kataoka*, H. Kamikubo**

16:40 – 1465. Genetically encoded electron transfer probes in proteins. **J. Wang**

Hawaii Convention Center
305A

Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403)

Organized by: A. Amirfazli, Y. Zuo, J. Li
Presiding: J.S. Allen, N. Gu, R. Veldhuizen, Y. Zuo

13:00 – 1466. Functional nanoparticles encapsulated lipid nanobubbles. **J. Tian, Y. Zhou, D. Sun, X. Lin, X. Ruan, F. Yang, N. Gu***

13:30 – 1467. Dynamics of high frequency ultrasound contrast agents. **J.S. Allen**

13:55 – 1468. Specific binding of functionalized droplets to integrin receptor $\alpha\gamma\beta_3$. **N.A. Smith, M.L. Fabilli, R. Seda, D. Li, J. Pitre, J.L. Bull**

14:15 – 1469. Phase transitions of biopolymers in cell-sized droplets coated with a lipid layer. **M. Yamagisawa***

14:35 Coffee Break

14:45 – 1470. Pulmonary surfactant: Drops, bubbles, and the lung. **R. Veldhuizen, J. Lewis, L. McCaig, F. Possmayer**

15:10 – 1471. Constrained drop surfactometer as a miniaturized film balance for studying spread and adsorbed films. **Y. Zuo***

15:35 – 1472. Interactions between inhaled particles and lung surfactant. **J.B. Sorli, E. Da Silva, S. Larsen**

16:00 – 1473. Surface free energy of bacterial cells: Determination and applications. **X. Zhang*, X. Zhang*, Y. Zuo***

16:25 – 1474. Impact of nanoparticles on the spreading of “living droplets”. **G. Beaune, F. Brochard-Wyart, F. Winnik***

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable, K. Liu, J. Lane, Y. Kajii, X. You
Presiding: X. You

13:00 – 1475. Key phenomena enabling direct simulation of real fuel combustion chemistry. **H. Wang**

13:30 – 1476. Predictive a priori kinetics for reactive intermediates. **S. Klippenstein*, N. Labbe, M. Verdicchio, K. Pelzer, M.P. Burke, C.F. Goldsmith, L.B. Harding, A. Jasper, A.M. Mebel, J.A. Miller, R. Sivaramakrishnan**

14:00 – 1477. Inelastic collisions between NO and NO₂. **E.A. Wade***, C. Sugie, D.W. Chandler, A. Jasper

14:20 – 1478. Reaction paths and intermediates in electrophilic aromatic substitution: New insights from experiment and theory. **S.A. Reid**

14:50 – 1479. Chemical activation in combustion and atmospheric chemistry. **P. Seakins***

15:20 – 1480. Non-adiabatic molecular dynamics simulations of isoprene photochemistry. **D.R. Glowacki*, B. Curchod, T.J. Martinez**

15:50 – 1481. Single-conformation vibronic and infrared spectra of alkylbenzyl radicals. **T.S. Zwier, J.R. Korn, K.M. Jawad**

16:20 – 1482. Predictive kinetic modeling of the pyrolysis and oxidation of cyclic molecules. **C.W. Gao*, W.H. Green**

16:40 – 1483. Muonium addition kinetics to alkenes and alkynes: the high-pressure limit at any total pressure?. **D.G. Fleming*, D.J. Arseneau, D. Garner, I.D. Reid**

Hawaii Convention Center
307AB

Recent Experimental and Theoretical Advances in Studies of Liquid Interfaces (#437)

Organized by: T. Tahara, A. Morita, R. Walker, L. Dang, H. Kang, S. Yamaguchi, J. Gibbs-Davis
Presiding: A. Morita, R. Walker

13:00 Opening Remarks

13:10 – 1484. Optical studies of competitive and cooperative adsorption to liquid interfaces. **R. Walker*, E. Gobrogue, L. Woods**

13:40 – 1485. Water flow along a solid surface affects interfacial water organization. **M. Bonn**

14:10 – 1486. Surface-bulk correlation spectroscopy of adsorbed biomass. **D. Horst***

14:40 – 1487. Structure and dynamics of water confined to nanoscale environments. **G.W. Leach*, A.K. Schiffer, A. Elliott, T. Johansson**

14:55 Break

15:15 – 1488. Single-channel heterodyne-detected sum frequency generation spectroscopy for liquid interfaces. **S. Yamaguchi**

15:45 – 1489. Spectroscopy and molecular orientation at aqueous interfaces. **A.V. Benderski**

16:15 – 1490. Unveiling microscopic structures of charged water interfaces by surface-specific vibrational spectroscopy. **C. Tian**

16:45 – 1491. Probing the buried interface between a tunable functionalized surface and aqueous solutions with heterodyned sum-frequency generation spectroscopy. **A.R. Barrett, M. McDermott, P.B. Petersen**

Friday Evening

Hawaii Convention Center
301B

Synergistic Relationships between Computational Chemistry and Experiment (#9)

Organized by: S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: K. S. Kim

19:00 – 1492. Alternative coupled cluster models. **G. Scuseria**

19:20 – 1493. Efficient computational methods for the accurate calculation of thermochemical properties. **B. Chan, L. Radom**

19:40 – 1494. Getting down to the fundamentals of hydrogen bonding: Anharmonic vibrational frequencies for hydrogen bonding prototypes from ab initio electronic structure computations. **G.S. Tschumper***

20:00 – 1495. Benchmarks for intermolecular interaction energies between larger systems. **T. Janowski, P. Pulay***

20:20 – 1496. Localized pair model of the chemical bond and non-covalent interactions. **A.J. Proud, B.H. Sheppard, J. Pearson**

20:40 – 1497. From chemical graph theory to the electronic structure fingerprinting of localization-delocalization matrices (LDMs) and of electron density-weighted adjacency matrices (EDWAMs). **C.F. Matta*, I. Sumar, R. Cook, P. Ayers**

Hawaii Convention Center
313B

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: A. Bertram, A. Laskin

19:00 – 1498. Hygroscopicity and mixing state of organics in atmospheric aerosols over Japan. **M. Mochida***

19:30 – 1499. Size distribution and mixing state of black carbon particles during a heavy polluted episode in Shanghai. **X. YANG**

19:50 – 1500. Chemical composition of marine clouds and fog in the Pacific and the Yellow Sea. **J.L. Collett*, T. Lee, A. Boris, D. Straub, K.B. Benedict**

20:10 – 1501. Photochemistry of individual particles: Evidence of sulfate formation through oxidation of organic sulfur compounds on particle surface. **S. Seng, Y. Tobon, R. Ciuraru, L.A. Picone, C. George, R.M. Romano, S. Sobanska**

20:25 – 1502. Understanding the effect of mixing state and water on CCN activation. **D. Vu*, S. Gao, M. Karabac, A. Asa-Awuku**

20:40 – 1503. Water adsorption on aerosols from nuclear magnetic resonance. **E. Vonhof*, F. Stratmann, M.S. Conrad, J. Haase**

Hawaii Convention Center
Halls I, II, III

Advances in Quantum Monte Carlo (#80)

Organized by: S. Tanaka, L. Mitas, P. Roy
Presiding: S. Tanaka

Poster Session

19:00 – 21:00

1504. Targeting excited states with quantum Monte Carlo. **L. Zhao, E. Neuscamman**

Hawaii Convention Center
Halls I, II, III

Recent Advances in Dynamics of Confined Liquids (#123)

Organized by: A. Luzar, G. Patey, M. Kinoshita
Presiding: M. Kinoshita

Poster Session

19:00 – 21:00

1505. Penetration of platinum complex anions into nanoporous silicon originating from surface-induced phase transition: Effect of counter cationic species.

A. Koyama, R. Koda, K. Fukami*, N. Nishi, T. Sakka, T. Abe, A. Kitada, K. Murase, M. Kinoshita

1506. Highly-efficient zinc electrodeposition within nanoporous electrodes: An effect of the ionic charge controlled by complexation. **Y. SUZUKI, A. Koyama, K. Fukami, A. Kitada, T. Abe, K. Murase***

1507. Solid-liquid and solid-solid phase transition of Lennard-Jones fluid in the confined 2D system. **H. Doi*, T. Kaneko, K. Yasuoka**

1508. Dynamics of supercooled water in partially crystallized gelatin-water mixture studied by broadband dielectric spectroscopy. **K. Sasaki*, R. Kita, N. Shinyashiki, S. Yagiura**

1509. Effect of charge density of ammonium cations on their penetration into nanoporous silicon electrodes. **Y. Imaoka, A. Koyama, K. Fukami*, A. Kitada, T. Abe, K. Murase**

1510. Interplay between thermomolecular orientation and imposed density gradients in models of confined fluids. **C.D. Daub*, J. Tafjord, S. Kjelstrup, P. Åstrand, F. Bresme**

1511. Destructive extraction of phospholipids from cell membranes by graphene nanosheets. **y. Tu**

1512. Characterization of ionic liquids between sliding surfaces using resonance shear measurement. **T. Kamijo, H. Arafune, T. Morinaga, T. Sato*, M. Hino, M. Mizukami, K. Kurihara**

1513. Exfoliation of electrolyte-intercalated graphene: Molecular dynamics simulations. **O. Lee***

1514. Bioinspired artificial single ion pump. **Y. Tian, L. Jiang**

Hawaii Convention Center
Halls I, II, III

Challenges in Plasmonic Photochemistry (#176)

Organized by: H. Misawa, P. Kamat, H. Sun, S. Gwo

Poster Session

19:00 – 21:00

1515. Effects of agglomeration of silver nanoparticles on refractive-index detection sensitivity. **Y. Takahashi*, Y. Yamaguchi, N. Ide, H. Tahara, T. Ishida, S. Yamada***

1516. Location, location, location: Distance dependant plasmon-enhanced singlet oxygen generation. **N. Macia, O. Planas, S. Nonell, B. Heyne***

1517. Edge-gold coated silver nanoparticles for efficient dielectric sensing and plasmon-enhanced organic photovoltaics. **C. Xue*, M. Shahjami**

1518. Selective nitrogen fixation to ammonia via plasmon-induced charge separation. **T. Oshikiri, K. Ueno, H. Misawa***

1519. Plasmon-mediated formation and growth of gold nanoparticles on ITO substrates. **S. Kajimoto*, T. Okamoto, T. Takahashi, H. Fukumura**

1520. Microfabrication of polystyrene quadrupole combined with top-down and bottom-up approach. **T. Takahashi, A. Matsutani, D. Shioji, K. Nishioka, T. Isobe, A. Nakajima, S. Matsushita***

1521. Ultrasensitive detection of chirality of viruses using chiral electromagnetic fields created by achiral metal nanostructures. **S. Hashiyada*, K. Karimullah, H. Okamoto, M. Kadodwala**

1522. Preparation and spectroscopic properties of gold nanoparticles modified with porphyrin monolayers. **T. Ishida*, Y. Takahashi, S. Yamada***

* Principle Author

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1523. Localized surface plasmon resonance induced visible light-responsive photocatalyst by loading (Au@Ag)@Au double shell NPs. **S. Yamashita**, S. Kamimura, T. Ohno*

1524. Plasmon excitation of size-controlled PbS quantum dots on Au/TiO₂ electrode for effective photocurrent generation at visible wavelength region. **X. Li***, K. Suzuki, T. Toda, S. Yasuda, K. Murakoshi

1525. Development of far-ultraviolet (FUV) surface plasmon resonance sensor using aluminum thin films. **T. Ryoki**, Y. Tanaka, I. Tanabe, T. Goto, . Kikawada, W. Inami, Y. Kawata, Y. Ozaki

1526. Exploring plasmonic hot spots and their dynamics by photoemission electron microscopy. **Q. Sun***, H. Yu, K. Ueno, A. Kubo, Y. Matsuo, H. Misawa

1527. In situ observation of enhancement of multiphoton emission from a single colloidal quantum dot (QD) using a silver-coated AFM tip. **H. Takata***, S. Masuo

1528. Development of metal-enhanced fluorescence platforms based on copper nanostructures. **K. Sugawa***, T. Tamura, H. Tahara, T. Akiyama, J. Otsuki

1529. Unique photocatalytic activity of Cu₂O/Cu plasmonic nanostructures under visible and near-infrared light. **N. Tsunenari***, S. Fujiwara, K. Sugawa, J. Otsuki

1530. Observation of charge separation between gold nanoparticles and titanium dioxide using surface plasmon spectroscopy. **X. Shi**, T. Oshikiri, K. Ueno, H. Misawa*

1531. Metal enhanced up-conversion fluorescence by triplet-triplet annihilation near silver nanoparticles. **S. Jin***, N. Takeshima, K. Sugawa, J. Otsuki

1532. Plasmon-enhanced surface catalytic coupling reactions of aromatic amine compounds. **M. Zhang**, L. Zhao, D. Wu*, B. Ren, Z. Tian

1533. Precise control of carrier density and thickness of thin film plasmonic solar cell. **K. Nakamura***, T. Katase, T. Oshikiri, K. Ueno, H. Ohta, H. Misawa

1534. Plasmon-induced photoelectric conversion system using gallium nitride substrate. **R. Masunaga**, T. Oshikiri, K. Ueno, H. Misawa

1535. Site-selective deposition of polypyrrrole via plasmon excitation. T. Toda, X. Li, H. Minamimoto, **K. Murakoshi***

1536. Spectral properties of plasmon-molecule hybrid states under strong coupling and its dynamics . **J. Li***, H. Uehara, T. Oshikiri, K. Ueno, H. Misawa

1537. Microscopic photoluminescence mapping of plasmonic enhanced emission from InGaN/GaN quantum well. **K. Tateishi**, **K. Okamoto***, M. Funato, Y. Kawakami, P. Wang, S. Ryuzaki, K. Tamada

1538. Biosensor fabricated by biomolecule-modified Au nanoclusters decorated TiO₂ photoelectrode. **J. Guo**, K. Ueno, T. Oshikiri, H. Misawa

1539. Fluorescence imaging of a single nanoparticle on the plasmonic chip. **K. Tawa***, C. Sasakawa, C. Hosokawa

1540. Spectral properties and dynamics of exciton-plasmon coupling states between Zn-aggregates and metal hybrid nanostructure. **H. Uehara***, J. Li, T. Oshikiri, Q. Chen, K. Ueno, H. Sun, H. Misawa

1541. Fano resonances on gold nano domes structures probed by photoemission electron microscopy. **H. Yu***, Q. Sun, K. Ueno, Y. Matsuo, A. Kubo, H. Misawa

Hawaii Convention Center
Halls I, II, III

Recent Progress in Matrix Isolated Species (#199)

Organized by: T. Momose, Y. Lee,
D. Anderson

Poster Session

19:00 – 21:00

1542. UV photochemistry of cyclohexadiene in solid parahydrogen. **J. Miyazaki***, S.Y. Toh, P. Djuricin, T. Momose

1543. Rotational and translational dynamics of hydrogen fluoride in solid parahydrogen. **S. Kumai***, Y. Miyamoto, H. Ooe, N. Sasao, K. Kawaguchi

1544. Matrix effects in NMR-matrix-isolation spectroscopy. **F.T. Zischka**, A.J. Kornath

1545. Exploring the potential energy landscape of alcohol-water complexes: The observation of large-amplitude hydrogen bond motion by far-infrared matrix isolation spectroscopy. J. Andersen, J. Heimdal, R. Wugt Larsen*

1546. Conformational properties and photochemistry of 2-(1,2,4-triazol-5(3)-yl)phenol in low temperature matrices.

M. Pagacz-Kostrewa*, M. Saldyka

1547. Photochemical reaction of sulfur hexafluoride with oxygen in low-temperature krypton matrices. **K. Iijima***, D. Takeda, Y. Yamada

1548. Isomerization and photodecomposition of N-hydroxyurea in argon matrices: FTIR and theoretical studies.

M. Saldyka*, M. Pagacz-Kostrewa

Hawaii Convention Center

Halls I, II, III

Metal Ions and Protein Functions: Theoretical Models and Applications (#202)

Organized by: Q. Cui, M. Meuwly, T. Allen, Y. Gao

Poster Session

19:00 – 21:00

1549. Catalase activity of Mn^{III} complexes. A. Romero-Rivera, **M. Swart***

1550. Computational study of effect of different metal ions on dioxygenase activity.

T. Saito, T. Numata, T. Kawakami, S. Yamanaka, M. Okumura

1551. Effects of salt ions on the dynamics and thermodynamics of protein unfolding and aggregation. H. Du, R. Jennings, Z. Liu, X. Qian*

1552. Modeling of ligand binding to metalloproteins. **A. Cho***

1553. New force field parameters for copper-zinc SOD1 enzyme and effects of SOD1 demetalation: Implications for understanding of the molecular origin of amyotrophic lateral sclerosis (ALS) and designing therapeutic targets for ALS treatment. **V.K. Hinge**, N. Blinov, N. Cashman, A. Kovaleko

1554. Structural elucidation of Ca²⁺-triggered folding in a de novo-designed intrinsically disordered peptide.

A.T. Church*, Z.E. Hughes, T.R. Walsh

Hawaii Convention Center

304B

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Eikerling, G. Jerkiewicz, S. Mitsushima, A. Gewirth
Presiding: H.H. Girault

19:00 – 1555. Ionic liquids in nanoconfinement and the physics of charging of nanoporous electrodes. **A.A. Kornyshev***

19:40 – 1556. Ultrathin carbon electrodes for molecular electronics. **R.L. McCreary***,

A. Bergren, B. Szeto, A. Morteza-Najaran, O. Ivashchenko, J. Fereiro, A. Bayat, D. James

20:10 – 1557. Studies of the electrodeposition of Ge and the possible formation of Germanene. **J.L. Stickney***

20:40 – 1558. Non-Faradic energy storage by room temperature ionic liquids in nanoporous electrodes. **D. Bedrov**, J. Vatamanu

Hawaii Convention Center
Halls I, II, III

Dynamical Intermolecular Interactions for Biological Functions (#307)

Organized by: D. Zhong, M. Terazima, Q. Lu

Poster Session

19:00 – 21:00

1559. Conformational dynamics of the cyanobacterial phycocrome1 (Cph1) studied by the transient grating method.

K. Takeda*, M. Terazima

1560. Photodynamic diagnosis of peritoneal metastatic cancer using photosensitizer Talaporfin in vivo. **H. Ryoma***, I. li

1561. Theoretical study of high-pressure effect on the structure of helical peptides.

Y. Mori, H. OKUMURA

1562. Insight into the binding domains of P-glycoprotein through homology modeling and molecular dynamics simulation.

R. Arenas*, Y. Ba

Hawaii Convention Center

305B

Photocatalysis and Charge Transfer at Interfaces and Nanomaterials (#344)

Organized by: D. Kilin, S. Kilina, I. Burghardt, G. Scholes, U. Diebold, A. Selloni, X. Gong, Q. Sun, R. Asahi, K. Donmen

19:00 Properties of Doped Titania Nano-structures

19:00 – 1563. Structural, electronic, and optical properties of minority surfaces, bilayers, and nanocomposites of anatase TiO₂: A combined DFT+MBPT analysis.

G. Giorgi, K. Yamashita

19:15 – 1564. Visible light-induced photocatalysis by rhodium-doped titania particles.

B. Ohnati*, T. Arima, M. Takase, J. Kunczewicz

19:30 – 1565. Visible light induced hydrogen evolution of alternate stacked structure of titanate nanosheets and tungstate nanosheets position-selectively modified with Pt complex and Ru complex.

F. Kishimoto*, D. Mochizuki, M. Maitani, E. Suzuki, Y. Wada

19:45 Plasmonic Nanoparticles for Photocatalysis

19:45 – 1566. Direct observation of plasmon-driven photocatalytic hydrogen generation over Au/Pt-TiO₂ composite nanofibers through dual-beam irradiation.

C. Xue, Z. Zhang

20:00 – 1567. Visible light photocatalytic performance of Au-Pd alloy nanoparticles for various reactions.

H. Zhu*, S. Sarina, Q. Xiao

20:15 – 1568. Novel photocatalyzed aqueous hydrogenation system for unsaturated aromatics using formic acid.

y. huang*, H. Zhu, C. Guo

20:30 concluding remarks

Hawaii Convention Center

Halls I, II, III

Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403)

Organized by: A. Amirfazli, Y. Zuo, J. Li

Poster Session

19:00 – 21:00

1569. Separation of chalcopyrite and pyrite through bioflootation. B. Breeze*, S. Harmer

1570. Preparation and hydrophobicity of solid/liquid bulk composite using porous glass and low-surface-energy oil.

K. Yokoyama, M. SAKAI, T. Isobe,

S. Matsushita, A. Nakajima*

1571. Phase-separated structures of mixed LB films of long-chain alcohol and hybrid carboxylic acid. **T. Sensui***, S. Watanabe, M. Matsumoto*, K. Murai

1572. Structure of Langmuir-Blodgett-Gibbs films of D19A and C12E8. **K. Suzuki***, S. Watanabe, K. Murai, M. Matsumoto

1573. Photoinduced manipulation of aqueous solutions using a photoresponsive surfactant. **Y. Ayako**, Y. Takahashi, Y. Kondo*

1574. Prevention of biofilm formation due to enzymatic inactivation of quorum sensing signal. **R. Kawakami**, Y. Takayama, Y. Sato, K. Iimura, E. Nasuno, N. Kato*

1575. Suppressive effects of cyclodextrins in biofilm formation of *Pseudomonas aeruginosa*. **Y. Sato**, R. Kawakami, K. Iimura, E. Nasuno, N. Kato*

1576. Aqueous phase behavior and polymerization of molecular assemblies in polymerizable gemini and monomeric surfactant mixtures. **N. Kobayashi**, Y. Takamatsu, T. Endo, K. Torigoe, K. Sakai, H. Sakai

1577. Preparation of polymer nanoparticle using highly stable oil in oil type emulsions. **A. Morioki**, T. Endo, K. Sakai, M. Abe, H. Sakai

1578. Emulsification by coacervate-type active interfacial modifier. **M. Tanaka**, T. Endo, K. Sakai, K. Sakamoto, M. Abe, H. Sakai

1579. Light-induced huge assembly formation, dense liquid droplets formation, and crystallization of protein at air/solution interface. **I. Yoshimatsu***, A. Miura, N. Kitamura

1580. Emulsification by poly(acrylic acid)-alkylamine complex as active interfacial modifier. **M. Shijo***, T. Endo, K. Sakai, K. Sakamoto, M. Abe, H. Sakai

1581. Selective formation of mannosyl-larabitol lipid by *Pseudzyma tsukubaensis* JCM16987. **A. Kosaka***, T. Morita, T. Imura, T. Fukuoka, K. Sakai, H. Sakai, M. Abe, D. Kitamoto

1582. Synthesis and interfacial properties of optical-active surfactants analogous to AOT. **S. Murooka**, Y. Takahashi, Y. Kondo*

1583. Detection of hydrogen nanobubbles at Pt(111) atomic flat surface. **K. Kashiwagi**, R. Shinohaki, S. Nakabayashi

1584. Fabrication of femtoliter polymer containers using droplets consisting of hydrocarbon oil/fluorocarbon oil. **M. Kano**, Y. Takahashi, Y. Kondo*

1585. Adsorption characteristics of vitamin A from its emulsion to lipid Langmuir monolayers. **M. Kawahara**, K. Iimura, M. Miyake

1586. Accurate measurement of surface viscosity for dilute surfactant monolayer with electromagnetically spinning system. **T. Hirano***, K. Sakai

1587. Measurement system for surface tension of flying droplet with high time resolution. **S. Mitani***, K. Sakai

1588. Study on existence inspection of the fine bubble. **T. Hata***, M. KARIYA, J. NAGAHARA, K. TADA, Y. NISHIUCHI, Y. YOSHIDA, S. WATANABE, M. OHMORI

1589. Colloidal stability of surfactant-free oil-in-water emulsions in multicomponent system. **A. YAMAMOTO***, T. Sakai

1590. Study on decomposition of organic matter by using the fine bubble and ultrasonic waves. **T. MORITA**, A. HIGUCHI, T. Hata*, J. NAGAHARA, K. TADA, Y. NISHIUCHI

* Principle Author

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- 1591.** Study on washing by using fine bubbles. **Y. MATSUDA**, T. ISHIZAKI, T. Hata*, J. NAGAHARA, K. TADA, Y. NISHIUCHI
1592. Study on oil/water (O/W) emulsion manufacture technology using liquid -liquid two phase flow. **K. TADA***, H. SURYADINATA, T. Hata, J. NAGAHARA, Y. NISHIUCHI

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable, K. Liu, J. Lane, Y. Kajii, X. You
Presiding: J.R. Lane

- 19:00 – 1593.** Reactions of atmospheric free radicals studied by cavity ringdown and time-resolved frequency comb laser spectroscopies. **M. Okumura***
19:30 – 1594. Imaging studies of atmospheric radical photochemistry: From energetics to roaming dynamics. **S.W. North**

- 20:00 – 1595.** Imaging the effect of reactant rotations on the dynamics of the Cl + CHD₃(v₁ = 1, |J, K>) reaction. **K. Liu***
20:30 – 1596. Zero-point energy corrected potential energy surface for roaming reactions. **M.J. Jordan***, K. Lee, S. Kable

Saturday Morning

Hawaii Convention Center
301B

Synergistic Relationships between Computational Chemistry and Experiment (#9)

Organized by: S. Wetmore, H. Ill, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: H. Nakai, J. Pearson

- 8:00 – 1597.** Fullerenes encaging metal atoms: Interplay of calculations and experiment. **S. Nagase**
8:20 – 1598. Playing with pentagons and hexagons: Fullerenes and their golden duals. **P. Schwerdtfeger***, L. Witz

- 8:40 – 1599.** DFT approaches designing new ferromagnetic organic magnetic diradicals. **J. Lee***, D. Cho, Y. Nam
9:00 – 1600. GPU-based molecular dynamics simulations of complex fluids and interfaces. **N.M. Cann**, S. Kazachenko, C. Si

- 9:20 – 1601.** Anisotropic noncovalent interactions in molecular assembly and collective properties in condensed phase. **K.S. Kim***
9:40 Break
9:50 – 1602. Dative bonding in main-group compounds. **G. Frenking***
10:10 – 1603. Molecular design of simple D-π-A architecture as potential sensitizers for highly efficient dye-sensitized solar cells. **S. Jungsuttiwong**

- 10:30 – 1604.** CompChem & NMR studies of quadrupolar nuclei in solution. **F. Moccia**, A. Laaksonen, M. Porcu, K. Aidas
10:50 – 1605. Theoretical studies of high pressure reactions. **N. Weinberg***, J.A. Spooner*, H. Wiebe*

- 11:10 – 1606.** Molecular dynamics of bimolecular organic reactions. **K.N. Houk***
11:30 Break

Hawaii Convention Center
306A

Coarse Grained Modeling and its Integration with Experiments (#30)

Organized by: R. Faller, D. Huang, M. Karttunen
Presiding: M. Karttunen

- 8:00 – 1607.** Molecular view on cellular membranes. **S. Marrink***

- 8:50 – 1608.** Insights into the packing switching of the EphA2 transmembrane domain by molecular dynamic simulations. **F. Sun***, S. Luu*

- 9:20 – 1609.** Computer simulations of membrane proteins in a plasma membrane model. **V. Corradi***, G. Singh, S. Marrink, D. Tielemans

- 9:50 – 1610.** Multiscale approach to protein-mediated interactions between cellular membranes: Using simulations of cadherin self-assembly to explain the experimentally observed sensitivity of the adhesion process. **A. Smith**
10:20 – 1611. Multiscale modeling with the integral equation coarse-graining approach. **M. Guenza**

Hawaii Convention Center
313B

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: E. Bieske, S. Nizkorodov

- 8:00 – 1612.** Complex refractive index of secondary organic aerosols generated from isoprene. **T. Nakayama***

- 8:30 – 1613.** Atmospheric processing of model mineral dust particles and the impact on aerosol optical properties. **M.A. Young**, J.M. Alexander, P.D. Kleiber, V. Grassian

- 8:50 – 1614.** Changes in the optical properties of secondary organic aerosols by chemical processes. **Y. Rudich***

- 9:20 – 1615.** Estimation of light absorption by biomass burning aerosols using detailed chemical composition data. **V. Sambourova**, M. Gyawali, R.L. Yatavelli, R. Chakrabarty, A. Watta, J. Knue, A. Cunningham, J. Connolly, H. Moosmuller, B. Zielinska, A. Khlystov*

- 9:40 – 1616.** Formation of light absorbing soluble secondary organics and polymeric particles from the dark mixing of catechol and guaiacol with Fe(III). **H.A. Al-Abadleh***, S. Slikoer, L. Grandy, S. Blair, S. Nizkorodov, R. Smith

10:00 Break

- 10:10 – 1617.** Cloud chamber studies of brown carbon formation and aerosol production by aqueous-phase aldehyde-amine reactions during cloud cycling. **D.O. De Haan***, M.D. Zauscher, L.N. Hawkins, A. Pajunoja, M. Cazaureau, E. Pangui, P. Formenti, J. Doussin

- 10:30 – 1618.** Brown carbon formation via atmospheric prevalent carbonyls reacting with methylpyrroles. **P. Lin***, P.K. Aiona, S. Nizkorodov, J. Laskin, A. Laskin*

- 10:45 – 1619.** Computational screening of possible brown carbon compounds in the atmospheric aerosol. **M. Caricato***

- 11:05 – 1620.** Molecular level characterization of aerosol nucleation processes - combined photoelectron spectroscopy and ab-initio modeling approach. **M. Valiev**, X. Wang

- 11:25 – 1621.** Molecular probe for SOA precursors: The photochemical mechanism of sunlight irradiated aqueous pyruvic acid. **A.J. Eugene**, M.I. Guzman*

- 11:40 – 1622.** Composition and photochemistry of biodiesel and diesel fuel SOA. **S. Blair**, A. MacMillan, G. Drozd, A. Goldstein, P. Lin, J. Laskin, A. Laskin, S. Nizkorodov*

Hawaii Convention Center
308B

Advances in Quantum Monte Carlo (#80)

Organized by: S. Tanaka, L. Mitas, P. Roy
Presiding: C.J. Umrigar

- 8:00 – 1623.** Going beyond single determinant trial functions for diffusion Monte Carlo calculations. **K. Jordan***

- 8:35 – 1624.** QMC using very large configuration interaction-type expansions. **A. Scemama***, E. Giner, T. Applencourt, M. Caffarel

- 9:10 – 1625.** Targeting excited states directly in quantum Monte Carlo. **E. Neuscamman***

9:45 Break

- 9:55 – 1626.** Brueckner-Goldstone quantum Monte Carlo. **S. Hirata***

- 10:30 – 1627.** Water clusters, ice, and bulk liquid: Improving ab-initio structure and energetics. **D. Alfe***

- 11:05 – 1628.** Ab-initio molecular dynamics by quantum Monte Carlo. **S. Sorella***

- 11:40 – 1629.** Path integral Monte Carlo method for Rényi entanglement entropies. **C.M. Hermann***, S. Inglis, P. Roy, R.G. Melko, A. Del Maestro

Hawaii Convention Center
308A

Conformational Dynamics of Biomolecules and the Biomolecule-Solvent Interface (#98)

Organized by: M. Nagaoka, D. Leitner, J. Straub, Y. Gao
Presiding: R. Elber, C. Hyeon

- 8:00 – 1630.** Conformation changes and water-protein interaction change for function of proteins. **M. Terazima***

- 8:30 – 1631.** Simple, yet powerful conformational sampling methodologies for proteins. **R. Harada**, Y. Takano, Y. Shigeta

- 8:50 – 1632.** Protein-solvent dynamical coupling in solution and in membranes. **D. Tobias***

- 9:20 – 1633.** Vibrational coupling of site-specific probe pairs for 2D IR studies of protein conformational dynamics. **M.J. Tucker***

9:40 Break

- 9:50 – 1634.** Modeling nanotoxicity: Molecular simulation of protein-nanoparticle interactions and their implications in nanomedicine. **R. Zhou**

- 10:20 – 1635.** Accelerated quasidynamics of biomolecules steered with 3D-RISM-KH mean solvation forces. **A. Kovalenko***, I. Omelyan

- 10:40 – 1636.** Exact milestoneing. **R. Elber***

- 11:10 – 1637.** Inhibition of amyloid formation by immunoglobulin light chain variable domain based on the analysis of structural fluctuations. **D. Hamada***, H. Tsutsumi, M. Nawata, C. Ota

- 11:30 – 1638.** Site-specific interrogation of protein conformational dynamics. **F. Gai**

Hawaii Convention Center
305B

Recent Advances in Dynamics of Confined Liquids (#123)

Organized by: A. Luzar, G. Patey, M. Kinoshita
Presiding: D.T. Limmer

- 8:00 – 1639.** From microscopic ion adsorption to macroscopic wettability alteration at solid-liquid interfaces. **F. Mugele***

- 8:30 – 1640.** Toward ab initio molecular dynamics simulations of electrochemical reactions at battery electrode interfaces. **K. Leung***

- 9:00 – 1641.** Harvesting atmospheric water with dewetted polymer surfaces. **C. Neto***, O. Al-Khayat, S. Thickett, D. Beck

9:30 break

- 9:45 – 1642.** THz time domain studies of water entrapped in micelles. **M. Havenith***

- 10:15 – 1643.** Dynamic responses in electric field-induced nanowetting. **D. Bratko***, D. Vanzo, A. Luzar

- 10:35 – 1644.** Molecular dynamics simulation of water between metal walls under electric field: Dielectric response and dynamics after field reversal. **A. Onuki**

- 11:05 – 1645.** Surface effects in nanofluidic energy harvesting. **D.J. Rankin**, D.M. Huang*

Hawaii Convention Center
313C

Challenges in Plasmonic Photochemistry (#176)

Organized by: H. Misawa, P. Kamat, H. Sun, S. Gwo
Presiding: S. Link, H. Misawa

- 8:00 – 1646.** Simultaneous evaluation of fluctuation in surface-enhanced resonance Raman scattering and surface-enhanced fluorescence using single silver nanoparticle dimers. **T. Itoh***, Y.S. Yamamoto, H. Tamaru, V. Biju, S. Wakida, Y. Ozaki

- 8:20 – 1647.** Plasmonic metal-semiconductor composites for solar energy harvesting. **N. Wu***

- 8:50 – 1648.** Plasmonic gold nanoparticles in the cancer cell: Following cell cycle, photothermal cell death, drug delivery dynamics, and efficacy. **M.A. El-Sayed***

- 9:20 – 1649.** Nanovortex fields formed by designed plasmonic structures. **K. Sasaki***, R. Takei, K. Sakai

- 9:40 – 1650.** Plasmon-induced artificial photosynthesis using gold nanostructured oxide semiconductor photoelectrodes. **H. Misawa***, Y. Zhong, T. Oshikiri, Y. Mori, K. Ueno

- 10:10 – 1651.** Hot-electron induced photocatalysis. **P. Nordlander***

- 10:40 – 1652.** Plasmonic vertical split-ring resonators for sensing and light manipulation. **D. Tsai***, P. Wu, W. Hsu, . Chen, Y. Huang, W. Tsai, C. Liao

- 11:10 – 1653.** Photochemistry in ultranarrow plasmonic gaps. **C. Tserkezis**, R. Esteban, D. Sigle, J. Mertens, L.O. Herrmann, J.J. Baumberg, J. Aizpurua

- 11:30 – 1654.** Single-particle absorption spectroscopy by photothermal contrast. **S. Link**

Hawaii Convention Center
310 Theatre

Challenges and Opportunities for Exascale Computational Chemistry (#184)

Organized by: J. Rice, W. Swope, A. Rendell, Y. Okamoto
Presiding: W. Swope

- 8:00 – 1655.** *A priori* prediction of chemical reaction mechanisms in complex systems based on quantum chemical molecular dynamics. **S. Irie***

- 8:30 – 1656.** Challenge of simulating crystallisation from aqueous solution: Prospects for exascale computation. **J.D. Gale**, P. Raiteri, R. Demichelis, M. De La Pierre, T. Ling, A.L. Rohr

- 9:00 – 1657.** Challenges to overcome in polymeric simulations. **M. Stevens**

- 9:30 – 1658.** Quantum simulations of heterogeneous materials. **G. Galli***

10:00 Break

- 10:15 – 1659.** Improving the performance of ab initio molecular dynamics simulations for actinide and geochemical systems with new algorithms and new machines. **E.J. Bylska***, W.A. de Jong, M. Jacquelin, D. Song, J. Weare

* Principle Author

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10:45 – 1660. Development of massive parallel code for quantum mechanical molecular dynamics simulations: DC-DFTB-K program. **Y. Nishimura**, H. Nishizawa, M. Kobayashi, S. Irie, H. Nakai*
11:05 – 1661. Real-time electron dynamics for excited-state simulations on exaflop supercomputers. **X. Andrade***, A. Correa

Hawaii Convention Center
304A

Quantum Fluid Clusters (#203)

Organized by: T. Momose, A. Vilessov, M. Choi
Presiding: F. Stienkemeier, A. Vilessov

8:00 – 1662. Superfluidity in helium droplets. **J.M. Eloranta***
8:35 – 1663. Superfluidity in finite-size helium systems: Critical Landau velocity and vortices. **M. Drabbe***
9:10 – 1664. Superfluidity of quantum clusters in confinement. **M. Boninsegni***
9:45 Break
9:55 – 1665. Interaction anisotropy and chaos in collisions of ultra-cold highly-magnetic atoms. **S. Kotchigova***
10:30 – 1666. Dynamics of helium droplets in a cryogenic electrostatic ion storage ring. **S. Kuma***, Y. Nakano, Y. Enomoto, T. Azuma
10:50 – 1667. Theoretical calculations of rovibrational spectra of small molecules inside helium clusters. **M. Lewerenz**
11:25 – 1668. Dynamics of trapped molecules. **P. Roy***, T. Zeng

Hawaii Convention Center
304B

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Eikerling, G. Jerkiewicz, S. Mitsushima, A. Gewirth
Presiding: M. Eikerling, K. Malek

8:00 – 1669. Simulating electric double layers using density functional theory based molecular dynamics. **J. Cheng**
8:20 – 1670. First-principles prediction of solvation energies and redox potentials in aqueous environments. **I. Dabo***
8:50 – 1671. Structure of electrode/electrolyte interfaces studied from first principles. **A. Gross***
9:20 – 1672. Electrocatalysis on model electrodes and modern DFT concepts: Experiment meets theory. **S. Brimaud***, R. Behm
9:40 Break
10:00 – 1673. Modeling heterogeneous photoelectrocatalysis from first principles. **E.A. Carter***
10:40 – 1674. Electrocatalysis from first principles: Mechanistic insights into the oxygen and CO₂ reduction reactions. **M. Neurock***
11:10 – 1675. Reversible potentials, bond strengths, and insertion reactions on electrocatalysts. **A. Anderson**
11:40 – 1676. Computational modeling for understanding electrochemical processes at the bio-nano interface. **I. Matanovic-Gonzales***, S. Babanova, P. Atanassov

Hawaii Convention Center
312

Quantum Coherence in Energy Transfer: General Open System Theory and Methods (#297)

Organized by: J. Cao, P. Brumer, J. Wu

8:00 – 1677. Quantum spectroscopy of photosynthetic complexes with entangled photons. **S. Mukamel***, F. Schlawin, K. Dorfman

8:35 – 1678. Influence of initial electronic coherent superposition on energy transfer and charge separation dynamics in PSII reaction center. **D.F. Coker**, P. Huo, M. Lee
9:10 – 1679. Vibrational coherence dynamics in multidimensional spectra with the optimized mean-trajectory approximation. **M. Alemi, R.F. Loring***
9:45 – 1680. Quantum mechanics of open systems with three classes of bath. **Y. Yan**
10:20 – 1681. First-principles simulation of open systems. **G. Chen***
10:55 – 1682. Open quantum walk approach to a transport problems in biological systems. **F. Petruccione**
11:30 – 1683. Quantum-induced vs. thermally-induced structural transitions in small and very large Lennard-Jones clusters. **V. Mandelsham***, I. Georgescu*, J. Deckman*, P. Frantsuzov*

Hawaii Convention Center
301A

Dynamical Intermolecular Interactions for Biological Functions (#307)

Organized by: D. Zhong, M. Terazima, Q. Lu

8:00 Introduction
8:05 – 1684. Electrostatics, hydrogen bonding, and dynamics in proteins. **S.G. Boxer***
8:35 – 1685. Significance of dynamic interaction between the BLUF photoreceptor PixD and its downstream factor PixE for controlling phototaxis in cyanobacteria. **S. Masuda***
9:05 – 1686. Structural dynamics of proteins using novel visible fluorescence probes. **H. Pan, J. Xu***
9:35 – 1687. Controlling reactivity by remote protonation of a basic side group. **E. Pines***
9:55 Break
10:10 – 1688. Structural and functional dynamics of the influenza M2 proton channel. **F. Gai**
10:40 – 1689. Molecular mechanism of H/ACA RNP-guided pseudouridylation. **X. Zhao***
11:10 – 1690. On the low photo-inactivation rate of bacteria in plasma. **J. Chen**, P. Rentzepis, T.C. Cesario
11:40 – 1691. Prehydrated electron, reductive DNA damage, and cancer initiation. **Q. Lu***, Y. Mei, Q. Zhang

Hawaii Convention Center
306B

Dissociation of Biomolecules in the Gas Phase for Structural Characterization (#352)

Organized by: S. Shin, R. Julian, K. Honma, K. Siu, S. Blanksby
Presiding: R. Julian, S. Shin

8:00 Opening Remarks
8:05 – 1692. Proposed nomenclature system for peptide ion fragmentation. **K. Siu**
8:25 – 1693. Ground and excited state chemistry of peptide cation-radicals in the gas phase. **F. Turecek***
8:50 – 1694. Collisional isomerization and dissociation of odd-electron peptide ions. **I. Chu**
9:10 – 1695. Gas-phase ion-electron and ion-photon reactions for biomolecular structural determination. **K. Hakansson***
9:30 – 1696. Efforts to make radical-driven peptide fragmentation mass spectrometry as a more practical laboratory tool. **H. Oh**
9:50 – 1697. Evaluation of a bifunctional TEMPO-active ester reagent for peptide structure analysis by tandem mass spectrometry. **M. Schaefer***, C. Ihling, F. Falvo, A. Sinz
10:05 Break
10:15 – 1698. Peptide fragmentation: Energies, structures, and mechanisms. **P.B. Armentrout**, A. Mookherjee

10:40 – 1699. Reactions of small sulfur-containing molecules with hydrated radical anions in the gas phase. **C.A. Siu***
11:00 – 1700. Evaluation of gas-phase ion activation strategies for ‘targeted’ and ‘global’ identification, characterization, and quantitation of microcystin peptides. **G.E. Reid***, T.J. Attard
11:20 – 1701. Probing the residue configuration in peptides based on the MS-fragment of Pd (II)-peptide complexes. **Y. Pan**
11:40 – 1702. Peptide UV-photodissociation - a statistical interpretation. **J. Moon***, M. Kim, S. Yoon

Hawaii Convention Center
305A

10:05 – 1718. Nanocapillary bridging as a new tool for binding of ultraflexible reconfigurable nanoparticle filaments and gel networks. **O.D. Velev***, B. Bharti, M. Rubinstein, A. Fameau

10:30 – 1719. Charge effects on surfactant bilayer dynamics. **R.D. Bradbury**, M. Nagao

10:50 – 1720. Photoinduced coalescence of oil droplets in emulsions prepared using photoresponsive surfactants. **Y. Takahashi***, N. Koizumi, Y. Kondo*

11:10 – 1721. Basic flows in thermocapillary-driven convection in free liquid film. **I. Ueno***, L. Fei, T. Tamura, T. Kaneko, D. Pettit

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: H. Guo, D. Xie, A. Brown

8:00 – 1703. Photochemical dynamics. **D.G. Truhlar**
8:30 – 1704. State-to-state photodissociation studies by VUV-VUV laser time-sliced velocity-map imaging method. **C. Ng**
8:50 – 1705. Geometric phase effects in non-adiabatic dynamics near conical intersections. **A. Izmaylov***
9:10 – 1706. Role of triplets in photochemical processes of molecules in solutions. **Y. Luo**
9:30 – 1707. Novel path-integral based dynamics for photochemistry. **N. Ananth***
9:50 Coffee Break
10:10 – 1708. CPUF: Probing multichannel reaction dynamics with chirped pulse microwave spectroscopy in uniform supersonic flows. **A. Suits***, C. Abeysekera, L. Zack, N. Ariyasingha, B. Joalland, B. Park, R. Field, I. Sims
10:40 – 1709. Isotopic effects in the O + O₂ exchange reactions by reactive quantum wavepacket method. **Z. Sun**
11:00 – 1710. Long-lived complexes in the F + H₂O and F + CH₃OH hydrogen abstraction reactions. **R. Continetti***
11:20 – 1711. Quantum interference effect observed in various properties of photofragments of simple molecules . T. Matsuo, **S. Yabushita**
11:40 – 1712. H + H₂ quantum dynamics using potential energy surfaces based on the XYG3 type of doubly hybrid density functionals. **X. Xu, N. Su***, J. Chen, Z. Sun, D. Zhang

Hawaii Convention Center
326B

Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (#403)

Organized by: A. Amirfazli, Y. Zuo, J. Li
Presiding: J. Hao, T. Lee, O.D. Velev, Y. Zuo

8:00 – 1713. Viscoelastic surfactant gels. **J. Hao***
8:30 – 1714. Partially fluorinated self-assembled monolayers having an inverted surface dipole. O. Zenasni, M.D. Marquez, T. Lee*

8:55 – 1715. Mechanism of action of additives for flocculation and dewatering of mature fine tailings revealed by molecular theory of solvation. **S. Ilushak**, S. Stoyanov, A. Kovaleko*

9:15 – 1716. Using densely packed, hyperbranched, hydrocarbon surfactants to generate low aqueous surface tensions comparable to those attained with fluorinated surfactants. **M. Sagisaka***, R. Soma, T. Narumi, A. Ohata, C. James, A. Yoshizawa, F. Guittard, J. Eastoe
9:35 – 1717. Dispensing carbon nanotubes and graphene nanoplatelets with surface free energy. **X. Zhang***, X. Zhang*, Y. Zuo*

9:55 Coffee Break

* Principle Author

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- 9:00 – 1732.** In situ sum-frequency vibrational spectroscopy of electrochemical interfaces. **W. Liu***
- 9:15 Break**
- 9:35 – 1733.** Water orientation and dynamics at surfactant and lipid interfaces. **J. Skinner***
- 10:05 – 1734.** Computational SFG analysis of organic liquid surfaces. **A. Morita***, L. Wang, T. Ishiyama
- 10:35 – 1735.** Hydrogen bonding structure and dynamics at the liquid/solid interface. **J. Karmes, I. Benjamin***
- 11:05 – 1736.** Understanding the rates and molecular mechanism of water-exchange around aqueous ions using molecular simulations. **I. deng***
- 11:35 – 1737.** Molecular theory of liquid interfaces. **A. Kovalenko***
- Saturday Afternoon**
- Hawaii Convention Center
301B
- Synergistic Relationships between Computational Chemistry and Experiment (#9)**
- Organized by:* S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: N. Mora-Diez, P. Schwerdtfeger
- 13:00 Break**
- 13:10 – 1738.** Automatic search of reaction pathways for complex reaction systems using the Global Reaction Route Mapping (GRRM) strategy. **K. Morokuma**
- 13:30 – 1739.** Protodeauration step in gold(I)-catalysed organic reactions. **B.F. Yates***, A. Ariafrad, S. Hashmi, R. BabaAhamdi, P. Ghanbari, N.A. Rajabi
- 13:50 – 1740.** Computational investigation into the oxo-transfer mechanisms of diseleneno-Mo and W complexes. **E. Bushnell***
- 14:10 – 1741.** Refining our understanding of the complex solution chemistry of copper coordination with cuprizone. **J.M. Pushie***, K.L. Summers, K.H. Nienaber, S. Caine, I.J. Pickering, G.N. George
- 14:30 – 1742.** Mechanistic understandings of catalytic meta-C–H bond activations. **Y. Wu***
- 14:50 – 1743.** Application of halogen bonding to organocatalysis. **M. Wong***
- 15:10 Break**
- 15:20 – 1744.** Computational investigations of 1,2-HX elimination reactions in competition with 1,1-HX elimination reactions from halocarbons - using experimental evidence to validate computationally-generated transition state geometries. **G. Heard**
- 15:40 – 1745.** Can noncovalent interactions trigger spontaneous heterolytic and homolytic bond cleavages? **M. Yanez***, O. Mo, I. Alkorta, J. Elguero
- 16:00 – 1746.** Inversion reactions on graphene nanoflakes. **A. Karton***
- 16:20 – 1747.** Modelling aqueous proton-transfer steps: The reaction of CO₂ with aqueous amines. **A. East**
- 16:40 – 1748.** HERON reaction of anomeric amides. **S.A. Glover**
- Hawaii Convention Center
306A
- Coarse Grained Modeling and its Integration with Experiments (#30)**
- Organized by:* R. Faller, D. Huang, M. Karttunen
Presiding: R. Faller
- 13:00 – 1749.** Wear process simulation of polymer brushes using coarse-grained molecular dynamics. **R. Takakuwa***, Y. Higuchi, N. Ozawa, Y. Tsujii, K. Kurihara, M. Kubo
- 13:30 – 1750.** Coarse-grained molecular dynamics simulation for fracture process of double-network gel. **K. Saito***, Y. Higuchi, N. Ozawa, M. Kubo

- 14:00 – 1751.** Self-rolled nanotubes with controlled hollow interiors by surface grafts. **E. Sim***, M. Han
- 14:30 – 1752.** Coarse-graining electrostatic interactions in molecular simulations of ionic systems. **D. Bedrov***, J. Vatamanu
- 15:00 – 1753.** Minimal, soft, coarse-grained models for polymer blends and copolymers: Successes and challenges. **M. Mueller**
- Hawaii Convention Center
313B
- Chemistry of Atmospheric Aerosols (#56)**
- Organized by:* A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: A. Laskin, X. YANG
- 13:00 – 1754.** Model simulations of stress induced biogenic VOC emissions. **A.B. Guenther***, D. Gu, H. Yu
- 13:30 – 1755.** Ozonolysis of unsaturated biogenic VOCs: Formation of H₂SO₄ through the reaction of Criegee intermediates with SO₂. **W. Mellouki**, A. Kukui, H. Chen, Y. Ren, V. Daele
- 13:50 – 1756.** Analysis of bonding patterns in Criegee intermediates. **S.S. Xanthreas***, E. Milordos
- 14:10 – 1757.** New photosensitized aerosol source at the ocean microlayer. **C. GEORGE**, P.A. Alpert, R. Ciuraru, S. Rossignol, L. Tinel, M. Passananti, S. Perrier
- 14:30 break**
- 14:40 – 1758.** Understanding chemistry of organic aerosols using high-resolution mass spectrometry. **J. Laskin***, A. Laskin, S. Nizkorodov
- 15:00 – 1759.** Atmospheric dimethyl sulfoxide oxidized to methanesulfonate on aqueous aerosol surfaces. **A.J. Colussi***, S. Ernati*, Y. Sakamoto, K. Hara, M. Hoffmann
- 15:20 – 1760.** Size-dependent molecular-level characterization of secondary organic aerosol from O₃ vs. NO₃ oxidation of monoterpenes. **J. Fry***, H. Kang, D. Draper, A. Laskin, J. Laskin
- 15:40 – 1761.** Effects of temperature and relative humidity on photochemistry inside secondary organic aerosol materials. **M.L. Hinks***, M. Brady, H. Lignell, M. Song, J. Grayson, A. Bertram, P. Lin, A. Laskin, J. Laskin, S. Nizkorodov
- 15:55 – 1762.** Uptake of organic nitrates into secondary organic aerosols during the ozonolysis of α -pinene. **V. Perraud***, A.C. Vander Wall, B.J. Finlayson-Pitts
- 16:10 – 1763.** Direct observation of chiral-selective surface reaction of limonene and α -pinene on solid surfaces. **L. Fu**, H. Wang
- Hawaii Convention Center
308B
- Advances in Quantum Monte Carlo (#80)**
- Organized by:* S. Tanaka, L. Mitas, P. Roy
Presiding: J.B. Anderson
- 13:00 – 1764.** Quantum Monte Carlo methods in curved spaces: Applications to molecular clusters. **E. Curotte***, M. Mella, S.E. Wolf
- 13:35 – 1765.** Diffusion quantum Monte Carlo approaches for studying rovibrational excited states. **A.B. McCoy***, J. Ford, Z. Lin, M. Marlett, A. Pettit
- 14:10 – 1766.** Quantum Monte Carlo simulations of confined rotors. **P. Roy***
- 14:35 – 1767.** Variable spins in electronic structure quantum Monte Carlo calculations. **L. Mitas***, C. Melton
- 15:00 Break**
- 15:10 – 1768.** Magnetism and spin transport in transition metal organometallic clusters. **I. Stich***
- 15:45 – 1769.** Application of quantum Monte Carlo methods in acidity studies. **N. Thellamurege***, M. Per
- 16:05 – 1770.** Variational quantum Monte Carlo with inclusion of pairwise molecular orbital correlations. **S. Tanaka***
- Hawaii Convention Center
313C
- Challenges in Plasmonic Photochemistry (#176)**
- Organized by:* H. Misawa, P. Kamat, H. Sun, S. Gwo
Presiding: P.V. Kamat, C.F. Landes
- 13:00 – 1788.** Applications of plasmon-induced charge separation. **T. Tatsuma***, H. Nishi, K. Saito, K. Akiyoshi
- 13:20 – 1789.** Study of molecules released from bacteria using SERS based on arrays of Ag-nanoparticle plasmonic hot-junctions. **Y. Wang***
- Hawaii Convention Center
310 Theatre
- Conformational Dynamics of Biomolecules and the Biomolecule-Solvent Interface (#98)**
- Organized by:* M. Nagaoka, D. Leitner, J. Straub, Y. Gao
Presiding: d. matyushov, T. Yamato
- 13:00 – 1772.** Visualizing protein structural dynamics by time-resolved X-ray diffraction. **S. Adachi***
- 13:30 – 1773.** Volume profiles for conformational changes in macromolecules and their mechanistic applications. **H. Wiebe***, N. Weinberg*
- 13:50 – 1774.** Application of 2D fluorescence lifetime correlation spectroscopy to elucidating conformational dynamics of biomolecules. **K. Ishii***, T. Taha
- 14:20 – 1775.** Theoretical study of the dynamic heterogeneity in protein conformational dynamics. **T. Mori***, S. Saito
- 14:40 Break**
- 14:50 – 1776.** Mapping allosteric signaling pathways of GPCRs. **C. Hyeon***
- 15:20 – 1777.** Revealing structural dynamics of GPCR signaling through atomic-level simulation. **R. Dror**
- 15:40 – 1778.** "It is water what matters:" THz absorption spectroscopy as a powerful tool to study biomolecular hydration. **M. Havenith***
- 16:10 – 1779.** Dynamics of biomolecule hydration, crowding, and preferential solvation probed with ultrafast 2D-IR spectroscopy. **K. Kubaych**
- 16:40 – 1780.** Hidden roles of Na⁺ in enzymatic activation of thrombin. **I. Kurisaki***, M. Nagayagi, C.E. Barberot, M. Nagao
- 17:00 – 1781.** Single molecule and super-resolution study of nuclear structure and dynamics. **y. sun**
- Hawaii Convention Center
310 Theatre
- Challenges and Opportunities for Exascale Computational Chemistry (#184)**
- Organized by:* J. Rice, W. Swope, A. Rendell, Y. Okamoto
Presiding: Y. Okamoto
- 13:00 – 1797.** Turning on micromachines: Activation of cytokine receptors and transport proteins. **A.E. Mark***
- 13:30 – 1798.** Molecular dynamics calculation study of entire poliovirus empty capsids using K-computer. **S. Okazaki***
- 14:00 – 1799.** Multiscale modeling and design of biological systems in ground and excited states. **U. Rothlisberger***
- 14:30 – 1800.** Role of exascale computing in the modeling of polymeric nanoparticles for drug delivery. **W. Swope***
- 15:00 Break**
- 15:15 – 1801.** How do we map molecular dynamics simulations to exascale computing resources? Rethinking the problem. **R. Walker**
- 15:45 – 1802.** Multi-petaflops DFT calculations of electronic structure and electron transport. **J. Bernholc**
- 16:05 – 1803.** Molecular dynamics simulation: At a crossroad between molecular biophysics and exascale computing. **X. Cheng**
- 16:25 – 1804.** Molecular simulation toward in silico screening of materials: Prediction of n-octanol/water partition coefficients using molecular simulation combined with the theory of solutions in the energy representation. **M. Kitabata***, T. Kawakami, I. Shigemoto, Y. Mitsuta, N. Matubayasi
- Hawaii Convention Center
304A
- Quantum Fluid Clusters (#203)**
- Organized by:* T. Momose, A. Vilesov, M. Choi
Presiding: J.M. Eloranta, W.E. Ernst
- 13:00 – 1805.** Microsolvation at 0.37 K: IR spectroscopic studies of aggregates in superfluid helium nanodroplets. **M. Havenith***

* Principle Author

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13:30 – 1806. Spectroscopy and photochemistry in superfluid helium nanodroplets. **A. Slenczka***

14:00 – 1807. Path integral simulation studies on quantum clusters. **S. Miura**

14:30 – 1808. Infrared laser spectroscopy and ab initio computations of OH-(D₂O)_N complexes in helium nanodroplets.

J.T. Brice, C.M. Leavitt, C.P. Moradi, **G.E. Doubterly***, F.J. Hernandez, G.A. Pino

14:50 Break

15:00 – 1809. Quantum molecular dynamics of doped helium clusters. W. UNN TOC, **N. Halberstadt***

15:30 – 1810. Excitation and ionization dynamics in helium nanodroplets.

F. Stienkemeier*, M. Mudrich, J. von Vangerow, A. LaForge, A. Clavardini, P. O'Keefe, Y. Ovcharenko, T. Möller, M. Drabbel, P. Piselli, O. Plekan, P. Finetti, M. Coreno, C. Graziosi, R. Richter, K.C. Prince, C. Callegari, M. Ziemkiewicz

16:00 – 1811. Dynamics in helium nanodroplets studied by ultrafast XUV and X-ray techniques. **O. Gessner**

16:30 – 1812. Controlling strong field ionization of clusters in nanodroplets. **J. Tiggesbaumer***

Hawaii Convention Center
304B

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Eikerling, G. Jerkiewicz, S. Mitsuhashima, A. Gewirth
Presiding: G. Jerkiewicz, M. UMEDA

13:00 – 1813. Role of well-defined surfaces in electrocatalyst design. **V. Stamenkovic***

13:30 – 1814. Electrocatalysis on well-defined (100) Pt-Ni, Pt-Ir and Pt-Ru model systems. **D. Guay***

14:00 – 1815. Oxygen reduction reaction activity and durability of well-defined Pt-M(111) single crystal surfaces.

R. Kawamura, M. Asano, Y. Bando, H. Watanabe, S. Takahashi, N. Todoroki, **T. Wadayama***

14:20 – 1816. Surface structures enhancing the activity for the oxygen reduction reaction on well-defined single crystal electrodes. **N. Hoshi***, M. Nakamura

14:40 Break

15:00 – 1817. Shape-controlled and shape-degraded metal alloy ORR nanocatalysts: Atomic-scale growth, structure, degradation, and reactivity. **P. Strasser***

15:30 – 1818. Electrochemical preparation of Pt and Pt-based catalysts for fuel cell applications. **H. Kim**, S. Bong, S. Woo

16:00 – 1819. Mechanism of CO electro-oxidation on polycrystalline Pt in alkaline media studied by surface-enhanced infrared absorption spectroscopy. J. Joo, M.T. Koper, **M. Osawa***

16:20 – 1820. Electrocatalysis of CO in solution on Pt electrodes investigated by scanning tunneling microscopy and DFT calculations. **J. Inukai***, D.A. Tryk

16:40 – 1821. Irrelevance of CO poisoning in methanol and formic acid oxidation on PtRu surfaces. D. Chen, **Y. Tong***

Hawaii Convention Center
312

Quantum Coherence in Energy Transfer: Nanoscale and Excitons (#297)

Organized by: J. Cao, P. Brumer, J. Wu

13:00 – 1822. Direct vs indirect exciton dissociation and recombination dynamics: Role of interfacial disorder and coherence. **E.R. Bittner***

13:35 – 1823. Charge transport mechanism in organic semiconductors. **Z. Shuai***

14:10 – 1824. Coherent exciton decay and transfer in nanostructure arrays. **X. Li**, D. Lingerfelt, A. Petrone

14:45 – 1825. Time-dependent wavepacket diffusive method and its applications to carrier quantum dynamics in materials. **Y. Zhao***

15:15 – 1826. Vibronic quantum coherence in nonequilibrium exciton dynamics. **M. Thorwart***

15:50 – 1827. Impacts of environmentally induced fluctuations on quantum mechanical mixtures in energy/charge transfers and 2D electronic spectra. **A. Ishizaki**

16:25 – 1828. Spectroscopy and topological phases for organic excitons. **J. Yuen**

Hawaii Convention Center
301A

Dynamical Intermolecular Interactions for Biological Functions (#307)

Organized by: D. Zhong, M. Terazima, Q. Lu

13:00 Introduction

13:05 – 1829. Protein dynamics and protein design for enzymatic catalysis. **S.D. Schwartz***

13:35 – 1830. Redox-driven proton pumps: Insights from computer simulations. **A.A. Stuchebrukhov**

14:05 – 1831. Contributions of protein dynamics on coupled transfer of electron and protein processes. **J. Gao**

14:35 – 1832. Probing electrostatics and conformational motions along the catalytic cycle of an enzyme. **S. Hammes-Schiffer**

14:55 Break

15:10 – 1833. Protein structure and dynamics-force field and polarization. **J. Zhang**

15:40 – 1834. Molecular recognition conjugated with structural fluctuation of protein, studied by the 3D-RISM/RISM theory. **F. Hirata**

16:10 – 1835. Effects of sequence and chemical modification on DNA structure and protein/DNA interactions. **Y. Gao**

16:40 – 1836. Transient dimerization and conformational dynamics of full-length phototropin from *Chlamydomonas reinhardtii*. **Y. Nakasone***, K. Okajima, S. Tokutomi, M. Terazima

Hawaii Convention Center
306B

Dissociation of Biomolecules in the Gas Phase for Structural Characterization (#352)

Organized by: S. Shin, R. Julian, K. Honma, K. Siu, S. Blanksby
Presiding: S. Blanksby, K. Honma

13:00 – 1837. Probing gas phase biomolecular structure via excitation energy transfer. **R. Julian***

13:20 – 1838. Expanding the capabilities of multidimensional tandem mass spectrometry for top-down proteomics and structural biology. S. Chen, **D.H. Russell***

13:45 – 1839. Collision induced unfolding of protein complexes: Current mechanisms and applications. **B. Ruotolo***

14:05 – 1840. Comprehensive analysis of protein glycosylation on proteins and implications in disease biomarkers and therapeutic production. **C. Lebrilla***

14:30 – 1841. Supercharging and activation of proteins in mass spectrometry. **E. Williams**, C. Going, A. Susa, Z.B. Xia

14:55 Break

15:05 – 1842. Experimental and theoretical studies of the porphyrin binding site on G-quadruplex thrombin-binding aptamer. **S. Shin**

15:25 – 1843. Influence of protonation vs. noncovalent interactions with alkali metal cations on the structures and glycosidic bond stability of DNA and RNA nucleosides. **M.T. Rodgers**, R. Wu, Y. Zhu, C. He, L. Hamilo

15:50 – 1844. Top-down electron capture dissociation mass spectrometry for deep sequencing of phosphoproteins. **Y. Ge***

16:10 – 1845. Laser desorption of nucleic acid components and their structural characterization by IR spectroscopy. **H. Saigusa**

16:30 – 1846. Molecular dynamics simulation of the strand break processes in model DNAs: Analysis of electron and energy transfer. **H. Kono***, N. Hishinuma, M. Kanno, Y. Kino, K. Akiyama

16:45 – 1847. Theoretical study of the binding of tetracationic porphyrin to thrombin-binding aptamer. **H. Kim**, D. Kim, Y. Rhee, S. Shin*

Hawaii Convention Center
305A

Advances in Quantum Dynamics from Spectroscopy to Reactions (#384)

Organized by: H. Guo, D. Xie, A. Brown

13:00 – 1848. Probing resonances in chemical reactions. **X. Yang***

13:30 – 1849. Hybrid approach for ultracold chemical reactions. **B. Naduvath***

13:50 – 1850. Untangling the energetics and dynamics of reactions of ground state silylidyne radicals with hydrocarbon molecules. **R. Kaiser***, T. Yang, B. Dangi, M. Head-Gordon

14:10 – 1851. Surface temperature effects in methane dissociation on Ni and Ir surfaces. **A. Utz**

14:30 – 1852. Mixed quantum/classical theory (MQCT) for rotationally and vibrationally inelastic scattering. **D. Babikov***

14:50 Coffee Break

15:10 – 1853. Direct dynamics simulations. From microsolvation to semiclassical theory. **W.L. Hase***

15:30 – 1854. Muon science: Providing unique tests of quantum mass effects in the chemical sciences. **D.G. Fleming***, S.L. Mielke, B.C. Garrett, D.G. Truhlar, H. Guo, J. Manz, T. Takayanagi

15:50 – 1855. Mode-specific vibrational enhancement in reactions of polyatomic molecules. **A. Mullin***

16:10 – 1856. Quantum manifestation of transition state control of state-to-state dynamics. **H. Guo***

16:30 – 1857. Quantum dynamics on “on-the-fly” diabatic states: Theory and applications to small hydrogen bonded clusters. **S.S. Iyengar***

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable, K. Liu, J. Lane, Y. Kajii, X. You
Presiding: Y.J. Kajii

13:00 – 1858. Characterization of reactive intermediates in the ozonolysis reactions of alkenes. **J. Zhang***

13:30 – 1859. Photoelectron spectroscopy and photochemistry of ozone cluster anions, O₃⁻(H₂O)_n, O₃⁻(Ar)_n, O₃⁻(C₂H₄)_n, and nitrous acid anion, HONO⁻.

J. Lehman, A.M. deOlivera, A.B. McCoy, **W.C. Lineberger***

13:50 – 1860. Photolysis of organic compounds in atmospheric aerosols.

S. Nizkorodov*, M.L. Hinks, M. Brady, H. Lignell, S. Blair, S. Epstein, S. Kim, C. Engelmann, D. Romonosky, N. Ali, M. Saiduddin, M. Wu, J. Lee, P.K. Aiona, A. MacMillan, K. Malecha, M. Song, A. Bertram, J. Grayson, P. Lin, A. Laskin, J. Laskin, R. Gerber, D. Shemesh

14:10 – 1861. Infrared detection of syn-ICH₂OO and the Criegee intermediates CH₂OO. **Y. Lee**

14:40 – 1862. Kinetics of simple Criegee intermediates at atmospheric conditions. **J. Lin***

15:10 – 1863. Free radical multiphase chemistry of organic aerosols. **K.R. Wilson**

15:40 – 1864. In-situ mass spectrometric detection of radical intermediates at the air-water interface. **S. Enami***

16:10 – 1865. Quantum mechanics/molecular mechanics (QM/MM) perspective of reactive intermediates and non-covalent interactions. **R. Crespo-Otero, K. Bravo-Rodriguez, E. Sanchez-Garcia***

16:30 – 1866. Secondary organic aerosol formation via the oligomerization reaction of Criegee intermediate in the ozonolysis of unsaturated volatile organic compounds. **Y. Sakamoto**, R. Rajima, S. Inomata, J. Hirokawa

Hawaii Convention Center
307AB

Recent Experimental and Theoretical Advances in Studies of Liquid Interfaces (#437)

Organized by: T. Tahara, A. Morita, R. Walker, L. Dang, H. Kang, S. Yamaguchi, J. Gibbs-Davis
Presiding: I. dang, J. Skinner

13:00 – 1867. Protons and hydroxides in amorphous solid water: Interfacial distribution and transport mechanism.

H. Kang, D. Lee, C. Choi, T. Choi, B. Sung

13:30 – 1868. Interfacial interactions between water, ions, and polymers that aid in water purification. **M. Chaudhari, S. Rempe**

14:00 – 1869. “First Principles” vibrational spectroscopy of water from many-body molecular dynamics. **F. Paesani***

14:30 – 1870. 2D sum frequency generation spectra at vapor/water interface: Molecular dynamics simulation study.

T. Ishiyama*, A. Morita, T. Tahara

14:45 Break

15:05 – 1871. 2D heterodyne-detected vibrational sum-frequency generation study of water interfaces. **T. Tahara**

15:35 – 1872. Ultrafast vibrational dynamics at mineral/water interfaces. **E. Borguet***

16:05 – 1873. Ultrafast excited-state dynamics at liquid-liquid interfaces. **G. Licari, C. Hsieh, E. Vauthey***

16:35 – 1874. 2D SFG provides molecular insights into aggregation of amyloid peptides on self-assembled monolayers. **A. Ghosh***, J. Ho, **M.T. Zanni***

Saturday Evening

Hawaii Convention Center
301B

Synergistic Relationships between Computational Chemistry and Experiment (#9)

Organized by: S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: M. Wong

19:00 – 1875. Computational simulation of molecules interacting with intense laser fields. **H.B. Schlegel***

19:20 – 1876. Dyson orbitals within equation-of-motion coupled-cluster formalism for wave function analysis and cross section calculations. **A. Krylov**

19:40 – 1877. The SMART cyberinfrastructure: Space-time multiscale approaches for research and technology. **V. Barone***

20:00 – 1878. Something for almost nothing? A computationally tractable approach to variational anharmonic frequencies for molecules, clusters, and materials. **D.L. Crittenden***, M. Sibaev

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20:20 – 1879. Recent advances in F12 molecular electronic structure theory.
S. Ten-no*

20:40 – 1880. Electron-pair distribution functions for electron correlation studies.
J.M. Ugalde*

Hawaii Convention Center
313B

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bieske
Presiding: E. Bieske, C. Ro

19:00 – 1881. Direct measurements of the time-evolving optical cross-sections of individual aerosol particles. **J.P. Reid***, M.I. Cotterell, R. Willoughby, A.J. Orr-Ewing

19:30 – 1882. Incandescence of trapped carbon nanoparticles. **E. Bieske***

19:45 – 1883. Polycyclic aromatic hydrocarbons transported from China to Japanese island in the East China Sea. **K. Miura**, X. Yang, X. Chen, F. Meng, K. Sato, A. Takami, S. Hatakeyama*

20:00 – 1884. Microdroplet and mass spectrometry tools for the study of liquid-phase photochemistry. **A. Trevitt***, P. Tracey, C. Hansen, B. Vaughn

20:30 – 1885. Whispering gallery modes in optically trapped aerosol particles. **T.C. Preston***

20:45 – 1886. Chemical reactions induced by collision of aerosol droplets. **J. Kohno***

Hawaii Convention Center
Halls I, II, III

Conformational Dynamics of Biomolecules and the Biomolecule-Solvent Interface (#98)

Organized by: M. Nagaoka, D. Leitner, J. Straub, Y. Gao

Poster Session

19:00 – 21:00

1887. Phase-resolved high-resolution broadband sum frequency generation vibrational spectroscopy of peptides and proteins at surfaces and in membranes. **L. Fu, H. Wang**

1888. Application of the 3D-RISM-KH molecular theory of solvation to study biomolecular interfaces. **N. Blinov***, A. Kovalenko

1889. Reaction mechanism of glycynamide ribonucleotide synthetase in the purine nucleotide biosynthetic pathway: QM/MM simulations combined with a minimum energy path search algorithm and a free-energy perturbation method. **N. Yamamoto**, G. Sampei, G. Kawai

1890. Application of fragment molecular orbital method for structure-based drug design. **K. Fukuzawa***, T. Watanabe, Y. Okiyama, H. Watanabe, T. Honma, Y. Mochizuki, S. Anzaki, S. Tanaka

1891. Benchmark for new fragmentation breaking peptide bonds. **M. Sakaguchi**, K. Fukuzawa, Y. Mochizuki

1892. Smaller 145th residue makes fluorescent protein nonfluorescent: Fluorescence lifetimes of enhanced yellow fluorescent protein (eYFP) Y145 mutants and H148 mutants. **H. Hosoi***, S. Hazama

1893. Protein interactions in and at the membrane: Computational predictions and their validation for the plexin family of single transmembrane receptors. **M. Buck***

1894. Gating mechanism of the calcium release-activated calcium channel: Insights from the pore flexibility. **H. Dong***

1895. P-loop conformation governed crizotinib resistance in G203R-mutated ROS1 tyrosine kinase: Clues from free energy landscape. **T. Hou, Y. Li**

1896. Conformational sampling by a novel replica exchange method: *tq*-REM. **M. Lee, J. Yoon, S. Jang, S. Shin***

1897. Advanced simulations of peptide adsorption at the aqueous titania interface. **A.M. Sultan***, L. Wright, Z.E. Hughes, T.R. Walsh

1898. Molecular dynamics analysis of reactant complex structure of lactone ring-opening reaction catalyzed by cyclodextrin. **S. Ito***, M. Takayanagi, M. Nagaoka

1899. Calculation of β -cyclodextrin and guest binding enthalpy and entropy: From thermodynamics to kinetics. **Z. Tang*, C. Chang**

1900. Role of water molecule on the reaction mechanism of CAL-B catalyzed ring-opening polymerization of β -lactam: A QM/MM study. **C.E. Barberot***, I. Kurisaki, Y. Suzuki, M. Nagaoka

1901. Theoretical analysis of the effects caused by incorporation of Trifluridine to DNA. **J. Koseki***, K. Tsunekawa, M. Konno, N. Nishida, K. Kawamoto, Y. Doki, M. Mori, H. Ishii

1902. Affinity of HIV-1 antibody 2G12 with monosaccharides: A theoretical study based on explicit and implicit water models. **K. Noto***, K. Takano

1903. Molecular docking of alkyl benzozquinones and alkyl phenols with the XIAP's BIR3 domain. **M.A. Hernandez**, I. Ortiz Verano, D.R. Muñoz Cendáles

1904. Diffusion of nanoparticles in semidilute polymer solutions: A modecoupling theory study. **N. Zhao***

Hawaii Convention Center
305B

Recent Advances in Dynamics of Confined Liquids (#123)

Organized by: A. Luzar, G. Patey, M. Kinoshita

Presiding: M. Heyden

19:00 – 1905. Thermoelectrokinetic energy conversion in liquid water microjets. **R. Savally**

19:30 – 1906. Electrokinetic flow of aqueous NaCl solutions in amorphous silica nanotubes. **C.D. Daub***, N.M. Cann, D. Bratko, A. Luzar

20:00 – 1907. Simulations of water and ion transport through model nanopores: The influences of water parameters and pore geometry. **L. Liu, G. Patey***

20:20 – 1908. Field-induced electro-osmotic diffusion of uncharged particles in water. **A. Smith***

20:40 Q & A

Hawaii Convention Center
304A

Quantum Fluid Clusters (#203)

Organized by: T. Momose, A. Vilesov, M. Choi

Presiding: W. Jaeger

19:00 – 1909. Reactions driven by metastable helium anions in doped helium nanodroplets. **P. Scheier***

19:30 – 1910. On the role of helium anions in helium droplet. **A. Mauracher***, S.E. Huber, A.M. Ellis, P. Scheier

19:50 – 1911. Rotation of quantum impurities in the presence of a many-body environment. **M. Lemeshko**, R. Schmidt

20:20 – 1912. Hydrogen clusters in helium droplets probed by methane infrared spectroscopy. **T. Momose**

20:50 Break

Hawaii Convention Center
304B

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Ekerling, G. Jerkiewicz, S. Mitsuhashima, A. Gewirth

Presiding: D. Guay

19:00 – 1913. Novel materials for an efficient electrocatalyst for oxygen reduction reaction: Insulating boron nitride nanosheet on an inert gold substrate. **K. Uosaki***, G. Elumalai, H. Noguchi, A. Lyalin, T. Taketsugu

19:30 – 1914. Unraveling the mysteries of active sites in non PGM catalysts. **S. Mukerjee***

20:00 – 1915. Group 4 and 5 metal oxide-based compounds as new non-platinum oxygen reduction electrocatalysts. **A. Ishihara***, K. Matsuzawa, S. Mitsuhashima, K. Ota

20:20 – 1916. Oxygen reduction electrocatalysis: Mechanism and the design of new catalysts. **A. Gewirth**, C.J. Barile, E. Tse

20:40 – 1917. Study of the nickel oxy-hydroxide formation and ethanol electro-oxidation reactions at low temperature in alkaline media. **J. van Drunen**, A.F. Barbosa, G. Tremeliosi-Filho*

Hawaii Convention Center
301A

Dynamical Intermolecular Interactions for Biological Functions (#307)

Organized by: D. Zhong, M. Terazima, Q. Lu

19:00 – 1918. 2D IR spectroscopy reveals the dynamics a β -sheet intermediate in type-Ii diabetes. **A.B. Serrano**, L. Tu, D. Raleigh, M.T. Zanni

19:30 – 1919. Elucidating excited state reaction pathways in photosensitive systems using femtosecond stimulated Raman spectroscopy. **Y. Wang, B.G. Oscar, W. Liu, L. Tang, L. Zhu, C. Fang***

20:00 – 1920. On "allosteric" regulation through dynamical intermolecular interactions between proteins and small molecules/cations: A molecular dynamics simulation study. **M. Nagaoka***

20:30 – 1921. Molecular dynamics simulations for oligomerization and disruption of amyloid- β fibril. **H. OKUMURA***

Hawaii Convention Center

Halls I, II, III

Advances in Quantum Dynamics from Spectroscopy to Reactions (#384)

Organized by: H. Guo, D. Xie, A. Brown

Poster Session

19:00 – 21:00

1922. Resonant two-photon ionization of terpenyl derivatives in the presence of cyclodextrins. **Y. Kasaba**, T. Takeshita, M. Hara

1923. Theoretical infrared spectra of deuterated PAHs: Astrophysical implications. **A. Pathak***, M. Buraghain, P.J. Sarre

1924. Theoretical investigation of isotope exchange reaction between several small organic molecules and tritium. **L. Dong**, L. Du, Z. Tan

1925. Theoretical study of photoisomerization between 1,3-cyclohexadiene and 1,3,5-cis-hexatriene. **A. Ota***, O. Kobayashi, S.O. Danielache, S. Nambu

1926. First-principles in-situ XAS simulation of chemical reaction at cathode-electrolyte interface in Li-ion batteries. **T. Tamura***

1927. Nonadiabatic ab initio molecular dynamics of uracil and 6-azauracil. **S. Takashima***, T. Murakami, S. Nambu

1928. Measuring and modeling the electronic structure of explosives at the explosive/air interface. **D. Farrow***, I.T. Kohl, H. Fan, R. Knepper, M. Marquez, S.P. Kearney, J.J. Kay

Hawaii Convention Center

Halls I, II, III

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable, K. Liu, J. Lane, Y. Kajii, X. You

Poster Session

19:00 – 21:00

1929. Acetone photodynamics: What the fragments tell us. **K. Lee***, K. Nauta, S. Kable

1930. Atmospheric chemistry of cis-3,3,3-trifluoro-1-chloro-propene (HCFO1233zd(Z)). **O.J. Nielsen***, M. Sulbaek Andersen, L. Andersen, T.J. Wallington

1931. Atmospheric chemistry of trans-3,3,3-trifluoro-1-chloro-propene (HCFO-1233zd(E)). **M. Sulbaek Andersen***, O.J. Nielsen, L. Andersen, T.J. Wallington

1932. MRCI study of ground state and low-lying states of Si₂. **A. Shah, D. Corey, A. Seitz, J. Song***

1933. Reaction models of the pyrolysis of hydrocarbons. **A. Jamal***, K. Morokuma

1934. Non-intrusive isomer specific detection of combustion intermediates via photoionization through Rydberg states. **F. Rudakov***, P. Weber

1935. Bimolecular cyclization reactions under single collision conditions: Formations of the benzyl radical and toluene. **B.B. Dangi**, D.S. Parker, T. Yang, R. Kaiser, A. Jamal, A.M. Mebel

1936. Spectroscopic evidence of jet-cooled p -methyl-alpha-methylbenzyl radical. **S.K. Lee**

1937. Computational challenges in investigations of elusive intermediates in combustion and atmospheric chemistry. **E. Papajak**, J. Zádor

1938. Alternative fate of formyl: Formic acid as a combustion intermediate. **M. Döntgen**, W.A. Kopp, K. Leonhard

1939. Direct kinetic measurement of the reaction of the simplest Criegee intermediate with water vapor. **W. Chao**, J. Hsieh, C. Chang, J. Lin*

1940. Investigating the role of pyrene on the oxidative capacity of the atmosphere. **A.L. Gomez**, K. Foster*

1941. Method to estimate the contribution of unidentified VOCs to OH reactivity: Ambient air, car exhaust, and plant emission. **S. Kato***, Y. Nakashima, Y.J. Kajii

1942. Development of an instrument for the measurements of gaseous glycol by broad band cavity enhanced absorption spectroscopy (BBC-EAS). **Y. Nakashima**, H. Tsurumaru, Y.J. Kajii

1943. Unimolecular reaction dynamics of atmospherically relevant α -keto carboxylic acids: Capturing hydroxycarbene intermediates. **S. Sutradhar**, A.K. Samanta, H. Reiser*

1944. Atmospheric chemistry of (CF₃)₂CHOCH₃, (CF₃)₂CHOCHO, and CF₃C(O)OCH₃. **F.F. Österström***, T.J. Wallington, M.P. Sulbaek Andersen, O.J. Nielsen

Hawaii Convention Center
Halls I, II, III

Recent Experimental and Theoretical Advances in Studies of Liquid Interfaces (#437)

Organized by: T. Tahara, A. Morita, R. Walker, L. Dang, H. Kang, S. Yamaguchi, J. Gibbs-Davis

Poster Session

19:00 – 21:00

1945. Molecular dynamics study of the structures at the free surface and the electrode interface of a quaternary ammonium based ionic liquid. **S. Kataoka***, N. Nishi, K. Kobayashi, K. Amano, T. Sakka

* Principle Author

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1946. Toward ab initio molecular dynamics modeling for sum-frequency generation spectra: An efficient algorithm based on surface-specific velocity-velocity correlation function. **T. Ohto***, K. Usui, Y. Nagata

1947. Vibrational spectroscopic study of lipid/water interface by molecular dynamics simulation. **D. Terada**, T. Ishiyama*, A. Morita*

1948. Heterodyne-detected vibrational sum frequency generation spectroscopy studies of hemocompatibility at the polymer/water interface. **A. Myaltsin**, S. Nihonyanagi, S. Yamaguchi, J. Yanagisawa, T. Aoki, T. Tahara*
1949. Nanoparticle-biomolecule interactions at aqueous interface investigated by surface-selective nonlinear spectroscopy. **Z. Lu***

1950. Reaction of SO_2 and NO_2 on ice surfaces at low temperature (90–170 K).

J. Bang*, Y. Kim, S. Kim, D. Lee, H. Kang
1951. Origin of the instability of octadecylamine Langmuir monolayer at low pH. **W. Sung**, Z. Avazbaeva, J. Lee, M. Phan, K. Shin, D. Vaknin, D. Kim*

1952. Developing ab initio-based potentials for studying ion hydration: The i-TTM model. **D.J. Arismendi Arrieta**, R. Prosmitsi, F. Paesani

1953. Non-uniform distributions of completely miscible liquids at gel/solid interface as probed by confocal Raman microscopy. **K. Honma**, K. Matsuka, M. Sano*

1954. Protein salting-out observed at a liquid interface. **Y.F. Yano***, E. Arakawa, W. Voegeli, T. Matsushita, T. Uruga

1955. Role of water fingering in ion transport through oil-water interface. **N. Kikkawa**, L. Wang, A. Morita*

1956. Heterodyne-detected vibrational sum frequency generation spectroscopic study on the structure of water at the air/water interface. **S. Nihonyanagi**, R. Kusaka, K. Inoue, A. Kundu, A. Adhikari, S. Yamaguchi, T. Tahara

1957. Eutectic mixture of indometacin and lidocaine can lower the entropy of fusion. **Y. Shimada***, H. Kataoka, R. Tateuchi, H. Terada, K. Makino, S. Gotou

1958. Transport properties of hydronium and hydroxide ions in amorphous solid water: Surface segregation and transport mechanism. **D. Lee**, J. Bang, Y. Kim, Y. Park, H. Kang*

1959. Characterizing the influence of interfacial environments on the early growth of *E. coli* biofilms. **T. Jarisz**, D. Hore*

1960. Enhanced understanding of amphiphatic peptide adsorbed structure by modeling of the nonlinear vibrational response. **S. Roy**, D. Hore*

1961. Thermodynamics and intrinsic structure of the Al–Pb liquid–liquid interface. **B.B. Laird**, Y. Yang

1962. Thermodynamics and kinetics for the particular phase transformation of S-ibuprofen/lidocaine mixture. **H. Kataoka**, r. tateuchi, Y. Shimada, S. Gotou

1963. Structure and oversaturation of the inclusion complex formed between 1,4-dihydropyridine calcium channel blockers and (2-hydroxypropyl)- β -cyclodextrin. **Y. Li**, Y. Shimada, Y. Yokoyama, . Terada, K. Makino, S. Gotou*

1964. Congo red aggregation and emulsion at the oil/water interface: A simplified model for histological amyloid aggregation. **T. Wada**, T. Iijima, S. Ososawa, Y. Shimada, S. Gotou

Sunday Morning

Hawaii Convention Center
301B

Synergistic Relationships between Computational Chemistry and Experiment (#9)

Organized by: S. Wetmore, H. III, L. Radom, P. Schwerdtfeger, R. Wah, H. Nakai, K. Kim
Presiding: J.M. Pushie, L. Radom

8:00 – 1965. “Negative” catalysis and cool quantum effects revealed through mutagenesis and quantum chemical studies of ornithine 4,5-aminomutase. **G. DiLabio***, K.R. Wolthers, C. Makins

8:20 – 1966. Catalysing alternate reactions to achieve high-fidelity: A multiscale computational study on aminoacyl-tRNA synthetases. **J.W. Gauld***

8:40 – 1967. Computing highly accurate spectroscopic line lists for characterization of exoplanet atmospheres and assign astronomical observations: A collaboration between theory and experiment. **T.J. Lee**, X. Huang, D.W. Schwemke

9:00 – 1968. Direct phosphorylation mechanism of GHMP kinases disclosed by hybrid QM/MM calculations. **M. Huang***

9:20 – 1969. Elongation factor 2 diphthamide unit: Unique, essential, and vulnerable. **L.A. Erikson***

9:40 – 1970. Computational insights into the development of novel therapeutic strategies for Alzheimer’s disease. **R. Prabhakar***

10:00 Break

10:10 – 1971. Applications of computer aided drug design to Alzheimer’s disease. **D.F. Weaver***, C. Barden, M. Reed, M. Taylor, F. Wu, E. Lu, A. Yadav, S. Yang, Y. Wang, L. Pan, M. Carter

10:30 – 1972. Comparing the binding strength of different pseudo-peptides to a model of amyloid beta peptide. **B. Mehrazma**, A. Rauk

10:50 – 1973. Competitive copper inhibiting ligands and protonation studies on $\text{A}\beta$ (13–23)/ligand design. **S.K. Opare***, A. Rauk

11:10 – 1974. Retired for 15 years and fretting over Alzheimer’s. **A. Rauk***

11:30 – 1975. Reflections of a computational quantum chemist on the road taken. **R.J. Boyd**

11:50 Break

Hawaii Convention Center
313B

Chemistry of Atmospheric Aerosols (#56)

Organized by: A. Laskin, S. Nizkorodov, A. Bertram, X. Yang, C. Ro, E. Bleske
Presiding: A. Laskin, S. Nizkorodov

8:00 – 1976. Latest developments in predicting aromatic-derived SOA in a regional air quality model. **M. Dawson**, R. Griffin, **D. Dabdub***

8:30 – 1977. Stochastic particle-resolved models for atmospheric aerosol simulation. **N. Riemer***, M. West

9:00 – 1978. New, experimentally based secondary organic aerosol paradigm. **A. Zelenyuk-Imre***, D. Imre, M. Shrivastava, J. Wilson, E. Abramson, J. Beranek, L. Kleinman, J. Fast, S. Springer

9:20 – 1979. Examination of sulfate aerosol formation over the southern ocean. **Q. Chen**, B. Alexander, Z. Xie, J. Dachs, J. Cole-Dai, L. Geng, M. Camp

9:35 – 1980. Simulating secondary organic aerosol and its climatic impacts from global to regional scales: Model improvements, multi-year applications, and interactions with climate. **Y. Zhang***, K. Yahya, T. Glotfelty, K. Wang

9:50 Break

10:00 – 1981. Mass spectrometric characterization and quantification of organosulfates in Chinese aerosols. **J. Yu***, B. Kuang, Y. Zhao, Y. Wang

10:30 – 1982. Effect of anthropogenic pollutants on biogenic organic aerosol formation. **J. Ye**, C. Adam, B. Urch, **A. Chan**

10:50 – 1983. Airborne submicron particulate. **J. Chen***

11:10 – 1984. Simultaneous measurements of aerosol metallic compositions at three Chinese and Japanese island sites.

S. Hatakeyama*, Y. Araki, K. Shimada, A. Yoshino, A. Takami, X. Yang, X. Chen, F. Meng

11:25 – 1985. Chemical composition of PM_{2.5} collected in São Paulo city, Brazil (2014). **P.C. Vasconcelos***, G.M. Pereira, S.E. Caumo, R. Hillamo, K. Saarnio, K. Teiniila, W. Maenhaut, M. Claeys

11:40 – 1986. Seasonal characteristics of PM_{2.5} components in urban environment, Busan, Korea. **G. Park***

Hawaii Convention Center
308B

Advances in Quantum Monte Carlo (#80)

Organized by: S. Tanaka, L. Mitas, P. Roy
Presiding: S. Tanaka

8:00 – 1987. Quantum Monte Carlo (QMC) simulation making progress for reactions at metal surfaces. **P.E. Hogan***

8:35 – 1988. Topological analysis of $|\Psi|^2$: Insight into chemical bonding with quantum Monte Carlo. **A. Luechow**

9:10 – 1989. Noncovalent interactions in molecules by quantum Monte Carlo. **M. Dubecky***

9:45 – 1990. QMC high performance computing of molecular interactions. **K. Hongo***, R. Maezono

10:05 Break

10:15 – 1991. Quantum Monte Carlo calculation of positron-attached polyatomic molecules. **M. Tachikawa**

10:50 – 1992. Quantum Monte Carlo calculations on helium clusters with open shell and ionic dopants. **M. Lewerenz**

11:25 – 1993. Atomistic quantum simulations of doped helium nanodroplets: Approaching the kilo-atom size regime. **R. Hinde**

Hawaii Convention Center
308A

Conformational Dynamics of Biomolecules and the Biomolecule-Solvent Interface (#98)

Organized by: M. Nagaoka, D. Leitner, J. Straub, Y. Gao
Presiding: M. Havenith, K. Kubarych

8:00 – 1994. Investigation conformational changes of biological macromolecules using kinetic network models. **X. Huang**

8:30 – 1995. Dynamic stabilization mechanism of human leukocyte antigen B*35: 01. **S. Yanaka***, T. Ueno, K. Tsumoto, K. Sugase

8:50 – 1996. Role of protein flexibility in immunogenic recognition. C. Ayres, B. Baker, S. Corcelli*

9:10 – 1997. Mechanism of quality control of biogenesis of OMPs in periplasm. **X. Zhao***

9:40 – 1998. Conformational dynamics coupled to signal transduction in downstream regulatory element antagonist modulator. **J. Miksovská***

10:00 Break

10:05 – 1999. Electron transport in biology: Ergodicity breaking and protein–water interface. **C. Matyushov***

10:35 – 2000. Interplay between interfacial water and signal transduction in proteins: Molecular dynamics study of virus-host protein complexes. P. Dutta, M. Bottani, S. Varma*

10:55 – 2001. Energy exchange network model of proteins. **T. Yamato***

11:25 – 2002. Oxygen behavior inside and surface of hemoglobin for respiratory function. **M. Takayanagi***, I. Kurisaki, M. Nagaoka

11:45 – 2003. Deciphering cryptic binding sites on proteins by molecular dynamics in mixed solvent. **S.R. Kimura**, H. Hu, A. Ruvinsky, A. Favia

Hawaii Convention Center
305B

Recent Advances in Dynamics of Confined Liquids (#123)

Organized by: A. Luzar, G. Patey, M. Kinoshita
Presiding: G. Patey

8:00 start 30 min later: 8:30 AM

8:30 – 2004. Nanoconfined catalytic Angstrom-size motors. **R. Kapral**, P. Colberg*

9:00 – 2005. Water in the pocket: Exploring local entropies and dynamics of water confined on biomolecular surfaces in atomistic simulations. **M. Heyden***

9:30 – 2006. Water dynamics and selective cation transport in ion channels and biological nanopores. **S. Noskov**, V. Ngo

10:00 break

10:15 – 2007. Macromolecular ion-solvent interactions in charged droplets. **S. Consta***

10:45 – 2008. Molecular dynamics simulation on the phase behavior of water confined in a periodic array of hydrophobic pillars. Z. Zhang, H. Kim, **J. Jang**

11:00 – 2009. GPU-accelerated replica-exchange molecular dynamics simulation of freezing behavior in confined quasi-1D water. **K. Nomura***, D. Takaiwa, J. Bai, K. Yasuoka, X.C. Zeng

11:15 – 2010. Solid-liquid critical behavior of water in hydrophobic nanotubes. **K. Koga**, K. Mochizuki

11:45 Closing remarks

Hawaii Convention Center
313C

Challenges in Plasmonic Photochemistry (#176)

Organized by: H. Misawa, P. Kamat, H. Sun, S. Gwo
Presiding: K. Murakoshi, H. Sun

8:00 – 2011. Fabrication of metal nanostructures using energy difference at organic/metal/dielectric interface. **S. Matsushita***, T. Sannomiya, T. Tatsumi, T. Takahashi, T. Isobe, A. Nakajima

8:20 – 2012. Identifying plasmons in molecular quantum-chemical calculations. **C.R. Jacob**

8:40 – 2013. Self-assembled metamaterials on a viral coat protein template. **A.S. Blum**, O. Zahr

9:00 – 2014. Control of multiexciton dynamics in a single quantum dot using plasmonic nanostructures. **S. Masuo***, H. Takata

9:20 – 2015. Plasmon-enhanced chemical oxidation of adenine adsorbed on silver nanostructures. **D. Wu***, R. Huang, Y. Chen, Z. Tian

9:40 – 2016. Protein-based functional micro-nano-devices enabled by femtosecond laser fabrication. **H. Sun**

10:10 – 2017. Broadband plasmonics toward high-efficiency light-emitting device. **K. Okamoto***, K. Tateishi, P. Wang, S. Ryuzaki, K. TANADA

10:30 – 2018. Ultrafast capture and release of hot plasmonic electrons in Ag@niobate nanopopepods. M. Liu, J.B. Wiley, P. Piotrowiak*

* Principle Author

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10:50 – 2019. Plasmonic photovoltaics at smooth and nanostructured metal/dielectric interfaces. **G.W. Leach***, F. MacNab, M. Cetinbas, C. McCague, H. Qiao, T. Johansson, X. Zhang, S. Gou, G. Wong, J. Chan, K. Khosravani, D. Star, A. Pattantyus-Abraham

11:10 – 2020. Surface plasmon resonance hydrogen sensing by electrons exchange. E. Gazzola, F. Romanato, M. Guglielmi, **A. Martucci**

11:30 – 2021. Characteristic intermediates at plasmon-induced water oxidation process. K. Suzuki, S. Yasuda, **K. Murakoshi***

11:50 Closing Remarks

Hawaii Convention Center
310 Theatre

Challenges and Opportunities for Exascale Computational Chemistry (#184)

Organized by: J. Rice, W. Swope, A. Rendell, Y. Okamoto
Presiding: A.P. Rendell

8:00 – 2022. Radical development of the fragment molecular orbital method. **D.G. Fedorov***

8:25 – 2023. Parallel implementations of multi-reference coupled-cluster methods for molecular systems. **K. Kowalski***

8:50 – 2024. Enhanced sampling methods for exascale computational chemistry. **Y. Okamoto***

9:15 – 2025. Ab initio predictions for structures and spectra of molecules in condensed phases. **S. Li**

9:40 – 2026. Concurrency and sparsity: Major challenges for electronic structure. **E.F. Valeev***

10:05 Break

10:20 – 2027. Accurate and robust embedding methodologies for enzymatic and catalytic systems. **J.D. Goodpaster***, T.F. Miller, A. Bell, M. Head-Gordon

10:45 – 2028. occ-RI-K: A fast, accurate new algorithm for exact exchange. **S. Manzer*, N. Mardirossian, P. Horn, M. Head-Gordon**

11:05 – 2029. Parallelization of quantum chemical calculations by using divide-and-conquer method. **T. Yoshikawa, H. Nakai**

11:25 – 2030. Linear-scaling quantum many-body theory via sparse scale-adaptive tensor algebra and massively parallel virtual processing. **D.I. Lyakh (Liakh)***

Hawaii Convention Center
304A

Quantum Fluid Clusters (#203)

Organized by: T. Momose, A. Vilesov, M. Choi
Presiding: T. Momose, J. Tiggesbaumer

8:00 – 2031. Modeling of soft, ⁴He droplet-assisted, deposition of metal nanostructures. **M. De Lara-Castells***, N. Aguirre, R. Fernández-Perea, C. Cabrillo, H. Stoll, A. Mitruschenkov, D. Mateo, M. Pi, L. Gómez, A. Vilesov

8:30 – 2032. Aggregation dynamics of metal dopants in helium nanodroplets. **W.E. Ernst***

9:00 – 2033. Cluster films by helium droplet mediated cluster assembly: growth and characterization. C.J. Ridge, S.B. Emery, K.B. Rider, **C.M. Lindsay***

9:30 – 2034. Helium nanodroplet spectroscopy of unstable species. C. Knapp, P. Das, **W. Jaeger**

10:00 Final remarks

10:10 – 2035. Ion-pairs in polar solvents: Infrared spectroscopy of salt-solvent complexes in helium nanodroplets. J. Tandy, A. Sadoun, G. Sarma, C. Feng, S. Yang, **A.M. Ellis***

10:40 – 2036. Effect of kinetic energy on the doping efficiency of cations into superfluid helium droplets. L. Chen, J. Zhang, W. Freund, **W. Kong***

11:10 – 2037. Symmetric arrangements of xenon clusters and quantum vortices in helium nanodroplets. **C.F. Jones***, R. Tanyag, C. Bernardo, L. Gómez, A. Vilesov, C. Bacellar, J. Cryan, K. Siefermann, F. Sturm, O. Gessner, D. Anileksi, L. Englert, L. Foucar, D. Rollés, A. Rudenko, J. Ullrich, R. Hartmann, K. Ferguson, S. Schorbar, C. Bostedt, F. Weise, S. Carron

11:30 – 2038. X-ray coherent diffraction imaging with superfluid helium nanodroplets. **A. Vilesov**

Hawaii Convention Center
304B

Molecular Perspectives on Interfacial Electrochemistry and Electrocatalysis (#218)

Organized by: M. Eikerling, G. Jerkiewicz, S. Mitsushima, A. Gewirth
Presiding: S. Mitsushima, P. Strasser

8:00 – 2039. Impact of temperature on platinum electro-oxidation and dissolution. **G. Jerkiewicz***, M. Alsabet, M. Grden, L. Xing, M. Hossaini, M. Tian, D. Beauchemin

8:20 – 2040. Electrochemical quartz crystal microbalance study of Pt electrode dissolution accelerated by H_2O_2 and Fe^{2+} in acidic solution. **S. SHIRONITA, M. INOUYE, M. UMEDA***

8:40 – 2041. Nanostructured porous electrocatalysts from modular templates. **B.D. Gates***, M.T. Paul, B.K. Pilapil, B. Yee, X. Zhang, D. Kim

9:00 – 2042. Electrolyte pore/solution partitioning under electric field. **D. Bratko***, F. Moucka, A. Luzzar

9:20 – 2043. New insights into the oxygen reduction reaction on platinum and platinum alloy surfaces. **D.A. Tryk***, M. Wakisaka, H. Uchida, M. Watanabe, A. Iiyama

9:40 Break

10:00 – 2044. Proton distribution at PTO/ionomer interface in the PEMFC catalyst layer model. A. Nouri Khorasani, K. Malek, M. Eikerling

10:20 – 2045. Microelectrode-based modeling of three-phase interface of polymer electrolyte fuel cell electrodes.

W. ZHANG, S. SHIRONITA, M. UMEDA

10:40 – 2046. How voltage drops are manifested by lithium ion configurations at interfaces and in thin films on battery electrodes. **K. Leung***

11:00 – 2047. First-principles modeling of electrolyte decomposition reactions on the spinel-structured $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ high-voltage cathode. **M. Olguín***, O. Borodin

11:20 – 2048. Coarse-grained molecular simulations of additives for secondary batteries. **H. Washizu***, K. Aikawa, T. Kinjo, H. Yoshida

11:40 – 2049. Development of noble-metal-based nanoreactors within mixed-metal oxide supports for efficient electrocatalytic oxidations of selected organic fuels. **I.A. RUTKOWSKA***, P.J. Kulesza*

Hawaii Convention Center
312

Quantum Coherence in Energy Transfer: Vibrational Dynamics and Dissipation (#297)

Organized by: J. Cao, P. Brumer, J. Wu

8:00 – 2050. New developments in the theory of dissipative systems. **E. Pollak***

8:35 – 2051. Steered quantum dynamics: Tunneling through Coulombic barriers and energy minimization. M. Soley, A. Markmann, **V. Batista***

9:10 – 2052. Quantum Brownian dynamics of open systems. **J. Shao***

9:45 – 2053. Effects of nuclear motion in an electronic energy-transfer system. **J.A. Cina***

10:20 – 2054. Gaussian process model of collision dynamics of complex polyatomic molecules. **R. Krems, J. Cui, Z. Li**

10:55 – 2055. Quantum energy flow and localization during photochemical reactions in proteins. **D.M. Leitner**

11:30 – 2056. Coherent nonlinear optical spectroscopy of interacting chromophores in optical cavities. **F. Herrera***

Hawaii Convention Center
301A

Dynamical Intermolecular Interactions for Biological Functions (#307)

Organized by: D. Zhong, M. Terazima, Q. Lu

8:00 Introduction

8:05 – 2057. Glucose binding and sensing using self-assemblies of boronic acid building blocks of peryleneimide framework. Z. Chen, X. Wu, Y. Huang, Z. Li, **Y. Jiang***

8:35 – 2058. Imaging neurodegeneration with coherent Raman contrast. **D. Cote**

9:05 – 2059. Cellular biochemical analysis and molecular imaging using laser tweezers Raman spectroscopy, reflectance confocal microscopy, and multiphoton fluorescence microscopy. S. Feng, Y. Huang, J. Zhao, E. Shen, Y. Tian, W. Wang, **H. Zeng***

9:35 – 2060. Molecular dynamics simulations on the interaction of the transmembrane NavAb channel with cholesterol and lipids in the membrane. C. Suwattanasophon, **R. Faller***

9:55 Break

9:55 – 2061. Recognition of bacterial protein biomarkers by synthetic DNA molecules. **Y. Li***

10:25 – 2062. Systematic study of protein dynamics by integrating click chemistry and mass spectrometry-based proteomics. **R. Wu***

10:55 – 2063. Urokinase receptor, a dynamic cell surface receptor capable to bind to different ligands. **M. Huang**

11:25 – 2064. Conformational influences of single-strand DNA on hybridization kinetics. **H. Hata, A. Suyama**

Hawaii Convention Center
306B

Dissociation of Biomolecules in the Gas Phase for Structural Characterization (#352)

Organized by: S. Shin, R. Julian, K. Honma, K. Siu, S. Blanksby
Presiding: P.B. Armentrout, K. Siu

8:00 – 2065. Combining ozone- with collision-dissociation for structure elucidation in complex lipids. **S. Blanksby**, T.W. Mitchell, M. Bhujel, D. Marshall, H. Pham

8:20 – 2066. Structural mass spectrometry strategies for comprehensive metabolomics – surface, electron, and collision dissociation information. **J.A. McLean**

8:45 – 2067. Unveiling lipid C=C location isomer distributions in biological samples using online photochemical reactions and MS/MS. **Y. Xia***

9:05 – 2068. Tandem mass spectrometry imaging of lipids and metabolites in tissue sections. **J. Laskin, I. Lanekoff, M. Thomas**

9:30 – 2069. Photodissociation spectroscopy of protonated histidine and its hydrogen-bonded clusters. **H. Ishikawa***, M. Kondo, Y. Kasahara

9:50 Break

10:00 – 2070. Spectroscopy of isolated ions in a RF ion-trap. **K. Honma**

10:15 – 2071. UV photodissociation of conformer selected protein ions. **G. von Helden**

10:40 – 2072. Flexible configurations of $\text{N}-\text{H} \dots \text{O}=\text{C}$ hydrogen bonds for pyrrole-ketone binary clusters studied by IR cavity ringdown spectroscopy. **Y. Matsumoto***, K. Honma

11:00 – 2073. Action spectroscopy of N-substituted azabenzenes ions: Product pathways and (some) vibronic structure. **A. Trevitt***, S. Blanksby, C. Hansen

11:20 – 2074. Cold spectroscopic study on metal ion-benzo-crown ether complexes in the gas phase. **Y. Inokuchi***

11:40 – 2075. Highly specific peptide-bond dissociation following exciting core electron of some peptide model molecules. **C. Liu***, Y. Lin, C. Ni

11:55 Closing Remarks

Hawaii Convention Center
305A

Advances in Quantum Dynamics from Spectroscopy to Reactions (#384)

Organized by: H. Guo, D. Xie, A. Brown

8:00 – 2076. Vibrational-induced steric effects on chemical reactivity. **K. Liu***

8:30 – 2077. State-to-state photodissociation dynamics of H_2O . **D. Xie**

8:50 – 2078. Ultraviolet photodissociation dynamics of the alkyl radicals. **J. Zhang***

9:10 – 2079. Sulfur mass independent fragmentation (S-MIF): How quantum dynamics will answer fundamental questions about the origins of life. **B. Poirier***, P. Kumar

9:30 – 2080. Further wrinkles on the photo-dissociation dynamics of acetone between 230 and 320 nm. **S. Kable***, M. Jordan, K. Lee, D. Andrews, K. Nauta

9:50 Coffee Break

10:10 – 2081. Photo-induced chemistry of Criegee intermediates. **M.I. Lester***

10:40 – 2082. Spectroscopy and dynamics study of Criegee Intermediate CH_3CHO . **X. Wang***, J. Bowman

11:00 – 2083. First-principles investigation of the electronic structure and dynamics of the photoexcited iodide-uracil complex. **C.C. Mak, G.H. Peslherbe**

11:20 – 2084. Single-conformation spectroscopy in the alkyl CH stretch region: Development of a first-principles model. **T.S. Zwier, D.P. Tabor, E.L. Sibert, N.M. Kidwell, D.M. Hewett**

11:40 – 2085. Theoretical study of ultraviolet induced photodissociation dynamics of sulfuric acid. **T. Murakami, S.O. Danielache, S. Nanbu***

Hawaii Convention Center
313A

Reactive Intermediates in Combustion and Atmospheric Chemistry (#419)

Organized by: D. Osborn, S. Kable, K. Liu, J. Lane, Y. Kajii, X. You
Presiding: K.R. Wilson

8:00 – 2086. Photodissociation of phenol derivatives, comparison of multimass ion imaging, velocity map ion imaging, and Rydberg atom translational spectroscopy. **C. Ni**

8:30 – 2087. Theoretical study on effect of water clustering on reactions: Dynamical and statistical aspect. **K. Takahashi**

9:00 – 2088. Water vapor enhancement of rates of peroxy radical reactions.

J. Hansen*, S. Kumbhani, T. Cline, M. Kilian, J. Clark, W. Keeton, L. Hansen, R.B. Shirts, D. Robichaud

9:20 – 2089. Simple model for the vibrational partition function to calculate the equilibrium constants for formation of peroxy radical/water complexes. **R.B. Shirts***, S. Kumbhani, E. Burrell, J. Hansen

* Principle Author

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9:40 – 2090. Concerted elimination vs. hydrogen migration in alkylperoxy radicals: The impact of tunnelling at low temperatures. A. Davis, J. Francisco*

10:10 – 2091. Novel technique for the determination of HOx yield from OH reaction in the atmosphere. Y.J. Kajii

10:40 – 2092. Laser-based field measurements of OH, HO₂, RO₂ and OH reactivity in the atmosphere and comparisons with numerical models. D. Heard*

11:10 – 2093. Gas phase reactions of alkyl amines in the atmosphere. T. Imamura*, K. Sato, T. Seta

11:40 – 2094. Atmospheric chemistry of tetrahydrofuran and lactones: Potential new biofuels. C. Andersen*, F.F. Østerstrom, M.P. Sulbaek Andersen, O.J. Nielsen

Hawaii Convention Center
307AB

Recent Experimental and Theoretical Advances in Studies of Liquid Interfaces (#437)

Organized by: T. Tahara, A. Morita, R. Walker, L. Dang, H. Kang, S. Yamaguchi, J. Gibbs-Davis
Presiding: J. Gibbs-Davis, T. Tahara

8:00 – 2095. Interactions of cations and anions at aqueous interfaces. P. Cremer*

8:30 – 2096. Specificity and variation of length scale over which monovalent halide ions neutralize a charged interface. W. Sung, W. Wang, J. Lee, D. Vaknin, D. Kim

9:00 – 2097. IV-SFG studies on the structure of liquid/liquid interface with a variation of phase boundary potential. Y. Ouchi*

9:30 – 2098. Ultrafast vibrational dynamics of water in the vicinity of positively charged interfaces studied by time-resolved heterodyne-detected vibrational sum frequency generation. P.C. Singh*, S. Nihonyanagi, S. Yamaguchi, T. Tahara

9:45 Break

10:00 – 2099. Counterfactual-enabled molecular spectroscopy from computation and experiment. F.M. Geiger

10:30 – 2100. Reorientation and intermolecular coupling of water molecules at the top-most layer of the air/water interface. H. Wang*

11:00 – 2101. Using nonlinear optical spectroscopy to monitor the relationship between water structure and the electric double layer at the silica/aqueous interface. J. Gibbs-Davis, A.M. Darlington, M. Azam

11:30 – 2102. Rearrangement of molecular orientation at liquid/superoleophilic interfaces and surfactant adsorbed human hair model interfaces probed by sum-frequency generation spectroscopy. T. Miyamae*

8:30 – 2. Prediction of MS signal intensities of pesticide transformation products over a range of analyte cation concentration basing on a novel ionization kinetic model of ESI with electrostatic field effects. T. Ueda*, H. Takanashi, J. Kadokawa

8:55 – 3. Optimization of dispersive liquid-liquid microextraction coupled with gas chromatography-negative ion chemical ionization mass spectrometry for the determination of pyrethroids in agricultural products. Y. Wang*, Y. Shu, J. Wang

9:20 – 4. Fast, sensitive technique for real-time, in situ quantification of commonly applied pesticides in the atmosphere using high resolution time-of-flight chemical ionization mass spectrometry. T. Murschell*, D. Farmer

9:45 Morning Break

10:00 – 5. United States survey of mycotoxins in beer, wine, cereal, milk, infant cereal, and infant formula by LC/MS/MS. J. Zweigenbaum, J. Cappozzo*

10:30 – 6. Mass spectrometry imaging of endogenous metabolites in *Arabidopsis*. T. Morikawa-Ichinose, J. Nakamura, Y. Fujimura, M. Shindo, H. Warishi, D. Miura*

10:55 – 7. Analysis and profiling of maple syrups by LC/Q-TOF-MS. I. Ferrer, M. Thurman, J. Zweigenbaum

Hilton Waikiki Beach
Prince David

NanoInterfaces and their Role in Environmental Systems and Processes (#86)

Organized by: D. Dionysiou, J. Gardea-Torresdey, W. Lee, X. Zhao, B. Pan, M. Litter
Presiding: D. Dionysiou

8:00 – 8. Electroreductive debromination of polybrominated diphenyl ethers by nitrogen-doped nanodiamond rod array electrode. X. Quan*, Y. Liu, S. Chen, H. Yu

8:30 – 9. Competing redox reactions at Fe²⁺-Cr³⁺-CeO₂ nanoparticle interfaces in wastewater treatment systems. J. Ray, Z. Li, C. Neil, B. Lee, Y. Jun*

9:00 – 10. Facile electrospinning of Pd-carbon nanofiber catalysts for waterborne contaminant reduction. D. Shuai, T. Ye

9:30 – 11. Formation of nitrous oxide (N₂O) hydrate in soil mineral suspensions with electrolytes. D. Kyung, T. Park, W. Lee*

10:00 Break

10:15 – 12. Interfacially electronic structures of gold-magnetite heterostructures for effectively reduction of nitrophenols. R. Doong*, S. Chang

10:45 – 13. Single particle characterization of the chemical reactivity and environmental transformation of nanoparticles using collision electrochemistry. A. Karimi, D. Andreescu, S. Andreescu*

11:15 – 14. Systematic development of oxygen reduction catalysts for water purification with molecular and materials design. J. Liu*, M. Han, X. Chen, T.J. Strathmann

Hilton Waikiki Beach
Territorial I & II

Sustainable Chemistry: Beyond the Bench (#103)

Organized by: M. Abraham, M. Gonzalez, P. Jessop, M. Hearn
Presiding: P.G. Jessop

8:00 Opening Remarks

8:05 – 15. Integrating metrics into sustainable chemistry research and development. D.C. Constable

8:40 – 16. Development of organic/inorganic composites formed through approaches inspired by biomineralization for functional materials. T. Kato*

9:15 – 17. Sustainability in the design and fabrication of a 3D-printed solid oxide fuel cell. G. Manoharan*, C. Linkous, M. Kioko, M. Abraham

9:40 Break - 15 mins

9:55 – 18. Application of flow chemistry to develop sustainable manufacturing in emerging countries. P. Watts*

10:20 – 19. Business logics for green chemistry. I. Milne*, S. Maguire

10:55 – 20. Chemical durability of pervious fly ash concrete under acidic environments. S.S. Hwang

Hilton Waikiki Beach
Kauai

UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204)

Organized by: G. Knight, W. Liu, K. Bell, M. Mohseni, K. Linden, G. Shin, K. Oguma
Presiding: K. Bell, G. Shin

8:00 Introduction to Symposium

8:05 – 21. Action spectra for pathogens and surrogates: Implications for polychromatic UV systems. S. Beck, K. Linden

8:35 – 22. Fundamentals of UV action of microorganism and the response (repair) of microorganism to UV action. G. Shin*

9:05 – 23. Molecular approaches to studying UV-induced damage of microorganisms. R.A. Rodriguez*

9:35 – 24. Implications of PCR techniques for measuring the fate of viruses and ARGs in UV-treated waters. K.R. Wigginton*, Z. Qiao

9:55 – 25. Impact of inner wall reflection on UV reactor performance as evaluated using the discrete ordinates (DO) radiation model. W. Li, M. Li, J. Bolton, Z. Qiang*

10:15 AM Tuesday Break

10:25 – 26. CFD models define advanced monitoring for polychromatic UV disinfection systems. H. Wright*

10:55 – 27. Communicating the science of UV to the regulatory and engineering community. K. Bell*

11:25 – 28. Sensing technology for validation and monitoring of disinfection at multiple wavelengths. G. Knight*, F. Daynour-Pancino, S. McDermid, B. Petri

Hilton Waikiki Beach
Prince Edward

Genomics and Metabolomics for Phytochemical Research (#267)

Organized by: K. Saito, E. Pichersky, V. Luca

8:00 Break (late start)

8:15 Introduction

8:20 – 29. Geranylinalool synthases and the origin of specialized terpenes in plants. E. Pichersky*

8:45 – 30. Genomic insight into gossypol biosynthesis in cotton. X. Chen*, C. Yang, Y. Mao, L. Wang

9:10 – 31. Discovery of a CYP450 for stereospecific monoterpenoid hydroxylation in thujone biosynthesis based on transcriptome and metabolite analysis of wildtype and mutant genotypes of *Thuja plicata*. J. Bohlmann, A. Gesell, M. Blaukopf, L. Madilao, M. Yuen, S.G. Withers, J. Mattsson, J. Russell

9:35 Coffee Break

9:55 – 32. Intriguing aspects of phenylalanine biosynthesis, regulation, and transport. N. Doudareva*

10:20 – 33. Melabolic profiling of isohexenyl-naphthalazins in *Echium plantagineum*, an exotic invader in Australia. D. Skoneczny*, P.A. Weston, G.M. Gurr, L.A. Weston

10:40 – 34. Dissection of pathway for prenylated polyketides. From glandular trichomes to chemical factory in yeast. G. Wang

11:00 – 35. Accumulation of chlorothalolinol in soil after repeated applications and its effect on soil enzyme activities and bacterial community structure. X. Wu, J. Tang, R. Hua, H. Cao, X. Li

Hilton Waikiki Beach
Hawaii

Phytochemicals for Crop Protection: Discovery to Molecular Target (#358)

Organized by: K. Matsuda, S. Duke, L. Weston
Presiding: S. Duke, L.A. Weston

8:00 Opening remark

8:05 – 36. Botanical insecticide pyrethrum elicits olfactory response in *Drosophila* antennae. K. Dong*, P. Xu, Y. Du

8:40 – 37. Deciphering biosynthesis of natural insecticides pyrethrins. K. Matsuda*

9:15 – 38. Phytochemicals as natural synergists to replace piperonyl butoxide (PBO) synergist in insect control. J.R. Coats, E.J. Norris, A.D. Gross, L.C. Bartholomay

9:50 Break

10:05 – 39. Grass roots chemistry: The development of meta-tyrosine, a non-protein amino acid produced by *Festuca* spp. as a potential commercial bioherbicide for weed suppression. L.A. Weston

10:40 – 40. Understanding the role of secondary metabolites in orchid pollination. R. Barrow*, B. Bohman, G. Flematti, P. Peakall, E. Pichersky

11:15 – 41. Probing the mode of action of natural phytotoxins with omics methods. S. Duke

11:50 Closing remark

Hilton Waikiki Beach
Prince Edward

Sources, Fates and Risks from Consumer Product Ingredients in the Environment (#391)

Organized by: P. DeLeo, K. Solomon, S. Mudge, C. Linares
Presiding: S. Mudge

8:00 Introductory Remarks

8:05 – 42. Effects of dissolved organic matter on the photochemistry of tricosan and triclocarban and the toxicities of their phototransformation products and mixture toxicities. K. Albanese, Y. Chin, R. Lanno, C.M. Hadad

8:35 – 43. Influences of ratios among elements from different sources on nitroamine formation during chloramination and ozonation of nizatidine and chlorphéniramine. W. Chen*

8:55 – 44. PBT 2.0? Perspectives on environmental assessment of consumer products and other industrial chemicals. B.W. Brooks

9:35 Break

9:50 – 45. Broad-scale exposure modelling and risk assessment of consumer product ingredients: Applications and opportunities using the iSTREEM® model. K.E. Kapo*, R. Vamshi, C.M. Holmes, P. DeLeo, D. Ferrer

10:30 – 46. Evaluation of anionic surfactants in the environment using a novel approach for regional probabilistic exposure assessments. K.M. McDonough*, T.W. Federle, K. Wehmeyer, S. Belanger, P. DeLeo

11:00 – 47. Fate of my fatty alcohol-based surfactants after changing the feedstock. S. Mudge

* Principle Author

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ENVR

Area 6 – Agrochemistry, Environmental and Geochemistry

Tuesday Morning

Hilton Waikiki Beach
Territorial III

Application of Mass Spectrometry to Agrochemical Challenges (#72)

Organized by: M. Thurman, Y. Wu, P. Marriott
Presiding: I. Ferrer, M. Thurman

8:00 – 1. Studies on advanced separations and detection methods for fatty acids and pesticides analysis in foods. P.J. Marriott, A. Zeng, S. Chin, X. Liu

TECHNICAL PROGRAM

Hilton Waikiki Beach
Molokai

Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400)

Organized by: M. Tunick, L. Liu, X. Liao, H. Nabetani, S. Yoon, X. Dai
Presiding: L. Liu, M. Tunick

8:00 Opening Remarks

8:05 – 48. Formulation and characterization of lipid-based micro/nanodispersion systems for developing food processing technology. **S. Ichikawa***

8:35 – 49. Characteristics and possible function of dehydrin proteins in crop seed. **M. Momma***

9:05 – 50. Fluorescence fingerprint for the rapid assessment of aging period of Awamori - the oldest spirits in Japan. **M. Tsuta*, E. Taira, M. Tsukahara, K. Tsukahara**

9:35 – 51. Polysorbate-false-positive substances in meat. **M. Ohnishi-Kameyama*, K. Takagi, I. Matsunaga, K. Kudo**

10:05 Break

10:20 – 52. Biobased, environmentally friendly lubricants for processing plants. **S.Z. Erhan, B.K. Sharma**

10:50 – 53. Anti-allergic action of 'Benifuuki' green tea rich in O-methylated EGCG and the use of new food functional labeling system in Japan. **M. Maeda-Yamamoto**

11:20 – 54. Using ultrahigh pressure treatment to stimulate the ageing process of wine. **X. Sun*, L. Li, X. Chen, W. Huang, J. Zhan**

Tuesday Afternoon

Hilton Waikiki Beach
Territorial III

Application of Mass Spectrometry to Agrochemical Challenges (#72)

Organized by: M. Thurman, Y. Wu, P. Marriott
Presiding: P.J. Marriott, J. Zweigenbaum

13:00 – 55. Simultaneous determination of acrylamide mercapturic acid adducts as short-term exposure biomarkers by isotope dilution ultra-high performance liquid chromatography coupled with tandem mass spectrometry. **Y. Zhang*, Q. Wang, J. Cheng, X. Chen**

13:30 – 56. Self-caramelization of sucralose: Identification of over 100 degradation products by UHPLC and LC/QTOF-MS with ultrahigh resolution time-of-flight mass spectrometry and accurate mass. **M. Thurman*, I. Ferrer, J. Zweigenbaum**

13:55 – 57. Determination of E,E-farnesol and squalene in Korean rice wine (makgeoli) using thermal desorption stir bar sorptive extraction coupled with GC-MS. **J. Ha*, H. Jang, J. Lee**

14:20 – 58. Mass spectrometry as the primary tool in the structure determination of agrochemical metabolites. **M.A. Jalal*, T. Nguyen, S. Bondarenko, R. Allen**

14:45 Afternoon Coffee Break

15:00 – 59. Direct simultaneous determination of 4-methylimidazole and 2-acetyl-4-(1,2,3,4-tetrahydroxybutyl)imidazole in vinegar by high performance liquid chromatography-electrospray ionization tandem mass spectrometry. **W. Rong**

15:25 – 60. Characterization of American elderberry fruit juice using mass spectrometry. **M. Johnson, A. Thomas, C. Greenleaf***

15:50 – 61. Mass spectrometric study of protoberryins in historical textiles dyed with *Kihada* (*Phelloendron* spp.). **Y. SASAKI, R. FUKAE, K. SASAKI**

16:15 – 62. Characterization of pyrrolizidine alkaloids in botanicals and dietary supplements by LC/QTOF MS. **B. Avula*, J. Zweigenbaum, S. Sagi, Y. Wang, M. Wang, I. Khan**

Hilton Waikiki Beach
Prince David

NanoInterfaces and their Role in Environmental Systems and Processes (#86)

Organized by: D. Dionysiou, J. Gardea-Torresdey, W. Lee, X. Zhao, B. Pan, M. Litter
Presiding: G. Li Puma

13:00 – 63. Redistribution of a protective alumina layer on sunscreen nanoparticles subjected to swimming pool and sea water. **S. Al-Abed***

13:30 – 64. Solar active nanocomposite photocatalysts for the removal of pharmaceuticals. **M. Kovacic, S. Salae, D. Juretic, H. Kusic***, U. Lavrenic Stangar, D. Dionysiou, A. Loncaric Bozic

14:00 – 65. Site-selective Pt-Pb nanoparticles deposition: TiO₂ nanorod photocatalyst for acetic acid oxidative decomposition under UV-VIS irradiation. **T. Tanabe*, W. Miyazawa, T. Gunji, S. Kaneko, M. Miyauchi, F. Matsumoto**

14:30 – 66. Highly efficient, visible-light-activated photocatalysts with post-illumination "memory" effect. **Q. Li**

15:00 Break

15:15 – 67. Achieving sustainable water treatment: Graphitic carbon nitride for persistent waterborne contaminant removal under visible light irradiation. **D. Shuai*, Q. Zheng**

15:45 – 68. Application of TiO₂ xerogel in coagulation. **S. Zhang, M. Li, X. Wang**

Hilton Waikiki Beach
Territorial I & II

Sustainable Chemistry: Beyond the Bench (#103)

Organized by: M. Abraham, M. Gonzalez, P. Jessop, M. Hearn
Presiding: M. Abraham

13:00 Opening Remarks

13:05 – 69. Life cycle impact assessment: What is the state of the research? **J.C. Bare**

13:40 – 70. Solvent wars: Sustainability awakens. **V. Isoni, L. Wong*, H. Khoo, P. Sharratt**

14:15 – 71. Virtual screening as a strategy for molecular design of switchable solvents. **J.R. Vanderveen, L. Patiny, P.G. Jessop***

14:40 Break - 15mins

14:55 – 72. Compatibility of green solvents with chemiluminescent labels. **J.-J. Grote**

15:20 – 73. Chemical properties and their impacts on the environment and functionality. **J.C. Bare**

15:45 – 74. Tailoring rhamnolipid and related glycolipid surfactant properties through sustainable production by green chemical synthesis. **J.E. Pemberton*, R. Palos-Pacheco, C. Coss, R. Gonzalez, L. Szabo, D. Hogan, F. Tian, R. Maier, R. Pot**

16:10 – 75. Chemistry and its role in sustainability. **M.A. Gonzalez***

Hilton Waikiki Beach
Kauai

UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204)

Organized by: G. Knight, W. Liu, K. Bell, M. Mohseni, K. Linden, G. Shin, K. Oguma
Presiding: K. Linden

13:00 – 76. Sunlight inactivation of viruses and bacteria: Mechanistic insights and implications for practice. **K.L. Nelson**

13:30 – 77. Photochemical (sunlight) fate of pharmaceutical compounds in natural waters and its application in the design and optimization of constructed wetlands. **W.J. Cooper**

14:00 – 78. Role of pH on photolytic and photocatalytic degradation of antibiotic oxytetracycline in aqueous solution under visible/solar light: Kinetics and mechanism studies. **C. Zhao*, H. Deng*, D. Dionysiou***

14:20 – 79. Model photosensitizers for the photochemical production of hydroxyl radical from dissolved organic matter. **G. McKay*, F. Rosario-Ortiz***

14:40 – 80. Looking at water chlorination in a new light: Mechanistic elucidation and modeling of enhanced microbial inactivation during solar photolysis of chlorine to reactive oxygen species and ozone. **P. Zhou, G.D. Di Giovanni, J.S. Meschke, M. Dodd**

15:00 Tuesday PM Break

15:15 – 81. Solar UV disinfection for water production in developing countries. **E.R. Blatchley***

15:45 – 82. Solar inactivation of fecal indicator bacteria and microbial source tracking markers in surface water. **A. Boehm*, M. Mattioli, L. Sassoubre, P. Maraccini, J. Griffith, Y. Cao**

16:15 – 83. Algal toxin photodegradation mediated by reactive halogen species in the marine environment. **K.M. Parker*, A. Ghadouani, W. Mitch**

16:35 – 84. Matrix effects in the attenuation of trace organics in wastewater effluent by solar irradiation. **L. Cheng*, T. Zhang, H. Vo, L.I. Márquez, D. Diaz, B. Dong, R.G. Arnold, E. Saez**

Hilton Waikiki Beach
Prince Johah

Genomics and Metabolomics for Phytochemical Research (#267)

Organized by: K. Saito, E. Pichersky, V. Luca

13:00 Break (Late start)

13:10 – 85. Biochemical basis of specialized metabolic evolutionary diversity: Acylsugars in the Solanaceae. **R.L. Last***

13:35 – 86. Genetic and structural variety of glycosyltransferases bring chemical diversity of flavonoids. **K. Yonekura-Sakakibara, K. Saito***

14:00 – 87. Expanding the toolbox for synthetic biology of tropane alkaloids. **J.C. D'Auria***

14:25 – 88. Evolution of lysine-derived alkaloid biosynthesis. **M. Yamazaki, S. Bunsupa, K. Saito**

14:50 Coffee Break

15:10 – 89. Combined genomics and metabolomics for phytochemical research in major crops. **J. Luo*, W. Chen, L. Gong, Y. Gao, X. Lian, Q. Zhang, J. Yan**

15:35 – 90. Integrated metabolomics, gene expression analyses, and GWAS identify saponin biosynthetic genes in *Medicago truncatula*. **L.W. Sumner, V. Tzin, J. Snyder, B. Watson, Z. Lei, D. Yang, Y. Tang, D. Nedveck, P. Tiffin, N. Young**

16:00 – 91. Metabolomics for heteroatom-containing metabolites in the case of sulfur-containing metabolites. **R. Nakabayashi*, Z. Yang, T. Nishizawa, T. Mori, K. Saito**

16:20 – 92. Integrated advanced multi-omics strategies: A new paradigm for agricultural and medicinal plant biotechnology with metabolomics/metabolite imaging *in situ*. **N.G. Lewis*, J.V. Marques, D.S. Dalisay, M.A. Costa, B. Herman, L.B. Davin**

Hilton Waikiki Beach
Hawaii

Phytochemicals for Crop Protection: Discovery to Molecular Target (#358)

Organized by: K. Matsuda, S. Duke, L. Weston
Presiding: S. Duke, L.A. Weston

13:00 Opening remark

13:05 – 93. Amaranthus toxicity in production livestock. **J.C. Quinn*, E. Birckhead, D. Skoneczny, A.E. Kessell, L.A. Weston**

13:35 – 94. Chemical ecology of three species of alien Orobancheae in Japan. **M. Morimoto*, M. Ishida, K. Matsuda**

14:05 Break

14:20 – 95. Discovery of novel targets for selective chemical control of root parasitic weeds based on metabolomic and transcriptomic analysis of their germination. **A. Okazawa*, T. Wakabayashi, T. Muranaka, Y. Sugimoto**

14:50 – 96. Discovery of plant chemical defenses and novel biosynthetic pathways. **M.C. Pedras*, Q. To, M. Alavi**

15:20 Closing remark

Hilton Waikiki Beach
Prince Edward

Sources, Fates and Risks from Consumer Product Ingredients in the Environment (#391)

Organized by: P. DeLeo, K. Solomon, S. Mudge, C. Linares
Presiding: K.R. Solomon

13:00 – 97. Estimating emissions and environmental exposure for home and personal care product ingredients at the global scale using spatially explicit data. **R. Vamshi*, C.M. Holmes, K.E. Kapo, J. Kilgallon, J. Hodges, O. Price, A. Franco, V. Slater**

13:30 – 98. High throughput modeling of exposures to semi-volatile chemicals in articles of commerce. **C.I. Nicolas*, M. Goldsmith, R. Pearce, R. Setzer, J. Wambaugh**

14:00 Break

14:15 – 99. Challenges of applying PBT criteria to super-hydrophobic chemicals used in consumer products: A case study of cyclic volatile methyl siloxanes. **D. Mackay*, D.E. Powell**

14:45 – 100. Assessment of the exposure and environmental health risks of siloxanes: The case of D5. **F.A. Gobas***

15:15 – 101. Quantitative weight of evidence analysis of the persistence, bioaccumulation, toxicity, and potential for long range transport of the cyclic volatile methyl siloxanes. **K.R. Solomon*, J. Bridges**

15:55 Closing Remarks

Hilton Waikiki Beach
Molokai

Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400)

Organized by: M. Tunick, L. Liu, X. Liao, H. Nabetani, S. Yoon, X. Dai
Presiding: L. Liu, M. Tunick

13:00 Opening remarks

13:05 – 102. Quality of whey powders stored under adverse conditions. **M. Tunick*, A. Thomas-Gahring, D. Van Hekken, S.K. Iandolo, R. Bazemore, C. Allison, K. Bazemore, M. Singh, P.X. Qi, D.O. Okuko, S. Mukhopadhyay, C.I. Onwulata, P.M. Tomasula**

13:30 – 103. Controlled delivery of 1-MCP from R₁, R₂-B-nethyle cyclopropane complexes: An effective approach to be used both in closed environments and open crop fields. **M.I. Sarker, P. Tomasula, L. Liu***

* Principle Author

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14:00 – 104. Quality changes of mango pulp after high pressure processing and high temperature short time. **X. Liao**
14:30 – 105. Protection of anthocyanins against acrylamide-induced oxidative stress. M. Zhao, J. Song, P. Wang, D. Li, F. Chen*

15:00 Break

15:15 – 106. Kinetic models for enzyme activity and thermo stability of polygalacturonase under ultrasound treatment. **D. Liu**

15:45 – 107. Oxidation of phytosterols in the model oil: Influence of heating and metal ions. **Y. Hu**, J. Deng, B. Lu*

16:10 – 108. Solar drying of papaya and pineapple from Fiji: Investigating nutritional and organoleptic properties of dried finished product. **R. RAJU***

16:35 – 109. Effects of processing units on secondary metabolites and functional properties of carrot juice processing. **T. Ma***, C. Tian, J. Luo, X. Sun, J. Zhan

Wednesday Morning

Hilton Waikiki Beach
Prince Edward

Ferrites and Ferrates: Chemistry and Applications in Sustainable Energy and Environmental Remediation (#13)

Organized by: V. Sharma, R. Doong, H. Kim
Presiding: R. Doong, J. Jiang, H. Kim, V. Sharma

8:00 Introduction

8:05 – 110. Application of ferrate(VI) to water treatment: Stability, kinetics, and mechanisms. **U. von Gunten**, Y. Lee

8:40 – 111. Advances of Ferrate(VI) preoxidation in water and wastewater treatment. **J. Ma**, Y. Liu, Z. Huang

9:15 – 112. Degradation of the cytostatic methotrexate by electrosynthesized ferrate (VI): Identification of oxidation by-products. **S. Barisci***, Ö. Türkay, F. Ulu, A. Dimoglo

9:40 Break

9:55 – 113. Oxidation of oseltamivir (or tamiflu) by ferrate(VI). **I. Lee**, Y. Hong, H. Kim*

10:20 – 114. Study on 4-bromophenol degradation using liquid ferrate(VI) synthesized by wet oxidation method. **F.B. Laksono**, I. Kim

Hawaii Convention Center
Halls I, II, III

Application of Mass Spectrometry to Agrochemical Challenges (#72)

Organized by: M. Thurman, Y. Wu, P. Marriott

Poster Session
10:00 – 12:00

115. Determination of emamectin benzoate and lufenuron in cabbage and soil under field conditions by QuEChERS and RRLC-MS/MS. **M. Hu**

Hilton Waikiki Beach
Prince David

NanoInterfaces and their Role in Environmental Systems and Processes (#86)

Organized by: D. Dionysiou, J. Gardea-Torresdey, W. Lee, X. Zhao, B. Pan, M. Litter
Presiding: W. Lee

8:00 – 116. Nanoparticle interaction with model biological membranes: Influence of lipid composition and non-lipid components. **J.A. Pedersen***, E.S. Melby, T.R. Kuech, I. Gunsulos, M.D. Torelli, A. Vartanian, G. Orr, C. Murphy, C.L. Haynes, R.J. Hamers

8:30 – 117. Disruption of critical growth and communication signals in bacteria: Nanoparticles that rescue cell populations. **K.B. Gregory***, E. McGivney, L. Han, J. VanBriesen

9:00 – 118. Effect of the substrate-bilayer interface on nanoparticle-induced membrane disruption of supported lipid bilayers. N. Yousefi, A. Wargenau, N. Tufenkji

9:30 – 119. Role of membrane proteins in nanoparticle interaction with supported lipid bilayers. **E.S. Melby**, A.C. Mensch, M.D. Torelli, L. Jacob, A. Vartanian, C. Murphy, R.J. Hamers, J.A. Pedersen

10:00 Break

10:15 – 120. Influence of environmental factors on nanoparticle-biological interactions and processes for disinfection. **S.O. Obare**, S.T. Nick, A. Bolandi

10:45 – 121. Extracellular polymeric substances reduced silver nanoparticles toxicity to wheat roots. **D. Zhou***

Hilton Waikiki Beach
Territorial I & II

Sustainable Chemistry: Beyond the Bench (#103)

Organized by: M. Abraham, M. Gonzalez, P. Jessop, M. Hearn
Presiding: M.A. Gonzalez

8:00 Opening Remarks

8:05 – 122. Removal of organic dyes and heavy metals from wastewater using new chitosan-based materials. **P. Champagne***, O. Garcia-Valdez, E. Madill, B. Tsai, M. Cunningham

8:30 – 123. Efficient multigram-scale synthesis of model lignin oligomers. **G. Sheldrake***, G. Forsythe, X. Ji

8:55 – 124. Definition and application of a sustainability indicator for the production of energy and carbon-based chemicals. **I.T. Horvath***

9:30 Break - 15 mins

9:45 – 125. From plant to plant - hydrothermal conversion of biomass. **A.K. Yuen**, T. Maschmeyer*

10:20 – 126. Vegetable proteins as potential carbon dioxide scrubbers. **G. Sun**, A. Aghanouri

10:45 – 127. Generation of anhydrosugars from carbohydrates by catalytic pyrolysis in dicotonic liquids. **G. Sheldrake***

Hilton Waikiki Beach
Territorial III

Chemistry and Biology of Auxin, Strigolactone and their Interactions (#107)

Organized by: T. Asami, Y. Zhao, C. Beveridge

Presiding: H. Kasahara, Y. Zhao

8:00 Preparation

9:00 Opening Remarks

9:05 – 128. How to make strigolactones. **S. Al-Babili***

9:45 – 129. Strigolactones as germination stimulants for root parasitic weeds. **Y. SUGIMOTO***, H. TAKIKAWA

10:15 – 130. Target sites for chemical regulation of strigolactone signaling. **H. Nakamura**, K. Fukui, O. Mashita, K. Kikuzato, T. Asami*

10:45 – 131. Regulation of strigolactone biosynthesis by gibberellin. **S. Ito**, D. Yamagami, M. Umehara, A. Hanada, S. Yoshida, S. Yajima, J. Kyozuka, M. Ueguchi-Tanaka, M. Matsuo, K. Shirasu, S. Yamaguchi, T. Asami*

11:05 – 132. Development of novel germination stimulant for *Striga*. **M. Yoshimura**, Y. Tsuchiya*, Y. Sato, K. Kuwata, A. Sato, S. Toh, D. Holbrook-Smith, H. Zhang, P. McCourt, K. Itami, T. Kinoshita, S. Hagiwara*

11:25 SL-BR Cross Talk

11:45 Lunch Time

Hilton Waikiki Beach
Kauai

UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204)

Organized by: G. Knight, W. Liu, K. Bell, M. Mohseni, K. Linden, G. Shin, K. Oguma
Presiding: G. Knight

8:00 – 133. Emerging UV technologies for fluid disinfection. **G. Knight***, F. Daynouri-Pancino, D. Bogovic

8:30 – 134. Novel deployment of UV-C LEDs in disinfection applications. **O. Lawal***

9:00 – 135. ACf cathode strengthen the E-UV-O₂ process to degrade nitrobenzene. **Y. Zhou***, Y. An, X. Zhang, X. Zhang, H. Zheng, C. Zhao

9:20 – 136. Disinfection and suspended solid reduction of municipal wastewater effluent by flow-through pulsed UV-light treatment system. **A. Demirci***, G. Uslu, J. Regan

9:40 – 137. Photobleaching of fulvic acid and oil sands blowdown water samples using chlorine oxidants and blue LED light sources. **M. Izadifarid**, C.H. Langford, G. Achari

10:00 Wednesday AM Break

10:10 – 138. UV light emitting diodes for water disinfection. **K. Oguma***

10:40 – 139. Optimizing pathogen inactivation at low energy cost with a tailored, multiple-wavelength UV LED unit. S. Beck, K. Linden

11:00 – 140. Plasma-based water treatment: An effective method to degrade perfluoroctanoic acid and other emerging contaminants. **S. Mededovic Thagard**, F. Dai, G. Stratton, C. Bellona, T. Holsen

11:20 – 141. Impact of fluence rate on microbial inactivation: Assessment with a novel minifluidic UV photoreaction system (MUPS). **M. Li**, W. Li, J. Bolton, Z. Qiang*

11:40 – 142. Liquid-phase electrical discharge plasmas for inactivation of microorganisms in water. **S. Rogers**, P. Estifaei, S. Mededovic Thagard

Hawaii Convention Center
Halls I, II, III

Genomics and Metabolomics for Phytochemical Research (#267)

Organized by: K. Saito, E. Pichersky, V. Luca

Poster Session

10:00 – 12:00

143. Development and application of a reporter bioassay system to screen for phytochemicals mimicking the anti-aging effects of caloric restriction. **T. Chiba**, Y. Ohata, Z. Wang, S. Serizawa, I. Shimokawa

144. Preventative effect of Hyuganatsu oranges on osteoporosis. **S. NISHIZONO***, H. Hata, Y. Sakatani, M. Yamaguchi, H. Sameshima

145. Serum metabolomics research of the antihypertensive effects of tengfu jiangya tablet on spontaneously hypertensive rats. **H. Jiang***, Y. Li*

Hilton Waikiki Beach
Hawaii

Environment and Gene Interaction (#336)

Organized by: G. Cobb, C. Matson, M. Hecker, C. Wong
Presiding: M. Hecker

8:00 Welcome and Introduction

8:05 – 146. Predicting consequences of xenobiotic-biomolecule interactions: Role of the adverse outcome pathway framework. **G. Ankley***

8:45 – 147. Environmental surveillance and monitoring – the next frontier for pathway-based high throughput toxicology. **D.L. Villeneuve***

9:15 – 148. Characterization of adverse outcome pathways of ethynodiol in *Xenopus laevis*. **M. Hecker**, A.R. Tompsett, S. Wiseman, E.B. Higley, J. Giesy

9:45 Break

10:00 – 149. Do differences in key amino acids in the aryl hydrocarbon receptor explain differences in sensitivity of fishes to dioxin-like compounds? **J. Doering***, S. Wiseman, R. Farmahin, S. Beitel, S. Kennedy, J.P. Giesy, M. Hecker

10:30 – 150. Impact of exposure to perfluoroalkyl acids on the development of metabolic diseases. **C.K. Wong***, R. Li, H. Wan

11:00 – 151. Interrelationships of microbial communities and secondary metabolite profiles from sponges around Okinawa Islands, Japan. **S. Aratake**, T. Fujii, M.C. Roy, T. Yamazaki, H. Jenke-Kodama

Hawaii Convention Center
Halls I, II, III

Phytochemicals for Crop Protection: Discovery to Molecular Target (#358)

Organized by: K. Matsuda, S. Duke, L. Weston
Presiding: K. Matsuda

Poster Session

10:00 – 12:00

152. Insect-antifeedant and growth-inhibitory activities of a limonoid from seeds of *Citrus reticulata* against larvae of Asian corn borer (*Ostrinia furnacalis*). **R. Abogado***, A. Abrera, M. Lit, M. Manalo

153. Phytotoxicity and insect antifeedant activity of calamene and cadinene type sesquiterpenes from camphorweed extract. **R. Morita**, M. Morimoto, K. Matsuda

Hilton Waikiki Beach
Prince Johah

Fukushima and Radiological Contaminated Environments World-wide: The Important Role of Environmental Chemistry and Radiochemistry in Remediation and Restoration (#374)

Organized by: T. Sasaki, H. Nitsche, C. Liu, Z. Yoshida, S. Kalmykov, L. Rao
Presiding: S.B. Clark, S.N. Kalmykov, T. Sasaki, Z. Yoshida

8:00 Opening remarks

8:05 – 154. Challenges for Fukushima environmental restoration - JAEA's perspective. **K. Iijima**, K. Miyahara*

8:45 – 155. ¹³⁴Cs and ¹³⁷Cs in the North Pacific Ocean derived from the TEPCO Fukushima Dai-ichi Nuclear Power Plant accident, Japan in March 2011. **M. Aoyama***

9:10 – 156. Sorption, diffusion, and migration of Cs-134/137, Sr-85/90 in loess: Laboratory and field experiments. **C. LIU***

9:35 Break

9:45 – 157. Experimental data and thermodynamic modeling of plutonium speciation in mineral colloidal suspensions. **A.Y. Romanchuk**, I. Vlasova, A. Egorov, Y. Zubavichus, S.N. Kalmykov

* Principle Author

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10:10 – 158. Accumulation of radioactive cesium in edible mushroom. **T. Ohnuki**, F. Sakamoto, N. Kozai, T. Saito, Q. Yu, S. Yamasaki

10:35 – 159. Application of bench-scale sample preparation techniques and 3D fluorescence for the speciation of Cs, Co and Cu in contaminated groundwater. **F. Caron***, S. Hume, S. Siemann

11:00 Break

11:10 – 160. Scientific aspects in development of the certified reference materials of fish meat and bone for determining radioactivity from FDNPP: Cs-134, Cs-137, and Sr-90. **Y. Minai***, T. Miura, C. Yonezawa, H. Iwamoto, M. Shibukawa, Y. Takagai, Y. Okada, M. Furukawa, F. Arakawa, K. Kakita, I. Kojima, Y. Uematsu, A. Okada, T. Sanada, T. Maeyama, T. Yamada, H. Ohta, S. Hirai

11:35 – 161. Radiocaesium fate in the Japanese agricultural systems and the effect of soil remediation acts. **K. Tagami***, S. Uchida

Hawaii Convention Center
Halls I, II, III

Sources, Fates and Risks from Consumer Product Ingredients in the Environment (#391)

Organized by: P. DeLeo, K. Solomon, S. Mudge, C. Linares
Presiding: P. DeLeo

Poster Session
10:00 – 12:00

162. Investigation of interactions between tribenuron methyl and montmorillonite: Insights on factors affecting its fate in soil. **S. Ahmadi***, F. Fathi, A. Ghasempour, M. Taghavi

163. An analytical method for simultaneous determination of alternative flame retardants of hexabromocyclododecane in indoors. **Y. Miyake***, H. Nakayama, T. Amagai, S. Ogo, K. Kume, T. Kobayashi, S. Takasu, K. Ogawa

Hilton Waikiki Beach
Molokai

Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400)

Organized by: M. Tunick, L. Liu, X. Liao, H. Nabetani, S. Yoon, X. Dai
Presiding: L. Liu, M. Tunick

8:00 Opening Remarks

8:05 – 164. Separation of benzoic acid from cranberry by use of nanofiltration.

H. Nabetani*, D. Quoc Lai, S. Hagiwara, N. Tagashira, T. Kimura, M. Nakajima

8:35 – 165. Review of current studies on radioactive cesium (^{134}Cs + ^{137}Cs) behavior in the processing and cooking of agricultural, livestock, and fishery products in Japan. **S. Kawamoto***, M. Hachinohe, S. Hamamatsu

9:05 – 166. Inactivation of spores in fruit juice and the quality change by high electric field alternating current. **K. Uemura***

9:35 – 167. Detection of novel trichothecene mycotoxin glucosides (masked mycotoxins) by high-resolution liquid chromatography-Orbitrap mass spectrometry.

H. Nagashima*, Y. Matsuo, H. Nakagawa

10:05 Break

10:25 – 168. Mitigation of acrylamide in potato chips in Japan. **M. Yoshida***

10:55 – 169. Formation and analysis of “food-borne toxicants”. **M. Granvogl**

11:20 – 170. Simultaneous determination of 113 pesticide residues in sorghum, rice husk, distilled spirit samples, and their dietary intake assessment. **y. han**, l. song, y. li, n. zou, y. qin, k. gu, j. zhang, c. pan*

Hawaii Convention Center
Halls I, II, III

Agrochemistry, Environmental, and Geochemistry General Posters
10:00 – 12:00

171. Comparison of *Cosmos bipinnatus* Cav. essential oil constituents in wild and cultivated population from Bangladesh and antimicrobial activity. **M.N. Bhuiyan***

172. Occurrence and source apportionment of pesticidal persistent organic pollutants in the surface riverine water from the eastern and northeastern part of India: Implications for ecotoxicological risk. **P. Chakraborty***, S. Khuman, S. Sakhivel, B. Kumar, L. Bommanra

173. Study on reduction of heavy metals in the foods using recycling resource. **J. Kim***, s. kweon, D. Heo, J. Kim

174. Classification of freshness using non-targeted analysis of volatile components, in frozen fishery products, during decay. **H. Park***, S. Lee, K. Um, A. Baek, J. Kim

175. Browning reduction of juice concentrate from a new cultivar of Asian pear (*Pyrus pyrifolia* cv. Hwasan) treated with different ascorbic acid concentrations. **J. Eun***, G. Jiang, S. Yim

176. Effects ofoxic and anoxic conditions on metals release from mine tailings. **S. Al-Abed**

177. Analysis of toxic metals leached into soils, water, and plants. **J. Chou***, J. Merono, T. Robinson

178. Standard heats of oxidation for soils in the remediation of chemically-contaminated soils and waters. **N. Moulton**, S. Mezyk, M. Becker

179. Thermodynamic analysis of Pb(II) and Ni(II) adsorption onto manganese oxide nanoparticles in the presence of humic acids. **S. Ko, B. Bae, A. Jang, S. Kang***

180. Modified dispersion property of carbon nanotubes hybrid photocatalyst containing both carbon nanotubes and titanium. **J.J. Bang***, S. Muslim, K. Kendall, c. Johnson, M. Nguyen

181. Effect of herbicide glyphosate on the cyanobacterium *Cylindrospermopsis raciborskii* growth and saxitoxin production. **F. Dorr***, E. Pinto

182. Monitoring and risk assessment of chemicals residues in commercial agricultural products in Korea. **A. Song***, J. Yim, S. Choi, J. Kim

183. Chlorophenol photodegradation in water from rural areas using carbon nanotubes and TiO₂ nanocomposites as photocatalysts. **S. Ponce***, J. Rodriguez, C. Belver, J. Bedia, A. Alvarez

184. Removal of diclofenac from water matrix by zeolite-assisted photo-AOPs. **D. Juretic***, H. Kusic, U. Lavrenic Stangar, D. Dionysiou, A. Loncaric Bozic

185. Sterilization with low temperature for long time in baby food added with persimmon (*Diospyros kaki* cv. Daebong) puree and citric acid. **J. Eun***, C. Lee, Y. Kim

186. Enhanced catalytic activity of doped graphene for wastewater treatment. **B. PARK***

187. Polycyclic aromatic hydrocarbons in the Japan Sea. **K. Hayakawa**

188. Utilization of raw and activated maize tassel for the removal of nutrient and heavy metal contaminants in water. **A.M. Shofolahan***

189. Sorption radioactive methyl iodide on silver doped zeolite for filtered venting system. **T. ISHII**, N. Sato, A. Kirishima, D. Akiyama, T. NARABAYASHI

190. Classification of almonds (*Prunus dulcis*) with concealed damage using near-infrared spectroscopy and partial-least square regression. **C. Rogel-Castillo***, R.B. Boulton, A.E. Mitchell

191. Plasmonic enhanced optical disk reactor for wastewater treatment. **M. Chen***, I. Chiang, W. Hsieh, Y. Chen, Y. Huang, C. Chu, D. Tsai

192. Leaching in soil column of Methiozolin. **J. Kim**, J. Kim, S. Kim, S. Choi, B. Lee, S. Koo, K. Hwang, J. Seo*

193. Debris plastics as sources of chemical contaminations of coast and open sea area. **K. Saido***, Y. Kodera, H. Sato, S. Togawa, N. Maximenko, K. Kogure, N. Togawa, D.M. Karl

194. Contamination by the styrene oligomer generated from debris polystyrene from coastal regions of Japan. **B. Kwon**, T. Kusui, A. Okabe, S. Chung, D.M. Karl, K. Takatama, M. Nishimura, **K. Saido**

195. Reactivity of horseradish peroxidase for detergent formulations. **M. Morita***, F. Masuko, K. Mase

196. Coastal phytoplankton growth in seawater media containing biodegradable chelating ligands and humic substances. **H. Hasegawa***, M.A. Rahman, M. Okada, T. Maki, Y. Tate, T. Ichijo

197. Removing diethylphthalate (DEP) from water systems by use of zeolites and mesoporous materials. **A. Masuda**, **H. Honda***

198. Antimutagenic activity of organic solvent extracts from pulp of *Pyrus communis* (pear). **H. Tomosaka***, S. Ota

199. Effect of 1-MCP treatment on quality and flavor of fresh-cut sage. **X. Zhao**, Y. Li, Y. Ma, C. Zhang

200. Removal of arsenic from aqueous solution using semi-burnt dolomite. **H. Sango***, M. Hirano

201. Chemometric analysis of real-time mobile membrane introduction mass spectrometry data for the source apportionment of atmospheric samples. **L. Richards***, D. Yeung, N. Davey, C.G. Gill, E.T. Krogh

202. Investigation of diarrhetic shellfish toxins using SPATT in Lingshan Bay, Yellow Sea, China. **z. li***

203. USP ● and you: What is the sum of toxic elements you might ingest every day?. **E.M. Pruszkowski**

204. Fruit polyphenols may play a role in fruit ripening and senescence. **W. Jiang***

205. Study on digestion of desiccated coconut and changes of pHs in simulated gastric acids. **H. Wu**, **J. Xiong**, **J. Ye***

206. Determination of the botanical origin of single-source honey samples and detection of adulteration with HFCS using SNIF (²D) NMR techniques. **A.D. Marchetti**, N.S. Green

207. Low temperature pyrolysis investigation on the behavior of hazardous materials in waste PCBs. **A. Shokri***

208. Isolation and characterization of plant growth promoting bacteria from earthworm. **N. Washio***, T. Ohike, M. Okanami, T. Aono

209. Improvement of a HONO sampling system and its application to atmospheric HONO monitoring in Vietnam and Japan. **H.T. Trinh***, N. Takenaka

210. Investigation of the catalyst for highly concentrated of ammonia and hydrogen peroxide removed in industrial wastewater by subcritical hydrothermal reaction. **M. Maeda**, D. Tokunaga, M. Negoro, A. Miyakoshi, K. Fukunaga, H. Yamasaki*

211. Removal of arsenic and lead from contaminated soils by washing with biodegradable chelating agents. **N. Jii**, H. Sawai, I.M. Rahmat, T. Maki, H. Ishiwata, H. Hasegawa

212. Antialgae activity of calcined colemanite. **H. Shoji***, A. Sato, H. Onami, A. Tsuneshige, S. Okouchi

213. Environmental geochemistry of tailing and stream water in Yonghwa Mine, Korea. **J. Kim**, Y. Kim, **H. Byun**, H. Jeon, J. Kim

214. Flu gas stream elemental mercury capture using activated carbon: A review. **S.R. Shewchuk***

215. Study of reductive reaction of selenite with hydrazine over metal oxide-supported Pt catalyst in aqueous solution. **J. Zhao**, H. Matsune, S. Takenaka, M. Kishida*

216. Optimization of dispersive liquid-liquid microextraction coupled with gas chromatography-negative ion chemical ionization mass spectrometry for the determination of nitrated polycyclic aromatic hydrocarbons in environmental aqueous samples. **Y. Shu***

217. Wound inducible antimicrobial compound in Citrus hassaku leaves.

T. Matsukawa*, T. Asai, S. Kajiyama

218. Characterization of the ACR12 gene in *Arabidopsis thaliana*. **M. Yoshizawa**, Y. Tanaka, M. Yamada, K. Sugiyama*

219. Study of cleaning effects in cleaning of microbubble with ultrasonic vibration considering environmental problem. **H. Ikeda***, K. Kurita, S. AOKI, S. HIRAI

220. Emission and behavior of Mercury, from the fumarolic activity of Minamijigoku-dani, Mt. Myoko, Japan.

H. Kodamatani*, S. Katsuma, A. Shigetomi, T. Hokazono, R. Imura, R. Kanzaki, T. Tomiyasu

221. Indium separation from lead-smelting dust by chelant-assisted extraction at high pressure and temperature.

H. Sawai*, I.M. Rahman, N. Jii, T. Wakabayashi, Z.A. Begum, T. Maki, S. Mizutani, H. Hasegawa

222. Novel adsorbent for removal of inorganic arsenic contained in polluted groundwater. **K. Inaba***, M. Haga, K. Ueda, H. Yoshikawa, T. Takemoto

223. Control of aqueous CO₂ concentration by temperature-sensitive materials for changing osmotic pressure. **J. Park**, Y. Lee*

224. Nondestructive prediction of degreening rate of broccoli buds by photosensing. **G. Amino**, Y. Makino*, S. Oshita

225. Microwave extraction of essential oil from Hyuganatu juice solid wastes. **K. Sugamoto**, N. Hirozawa, Y. Matsushita

226. Oxidation of trichloroethylene by persulfate activated with ZVMS. **Y. Kim***, J. Kim, J. Geum

227. Removal of toxic mercury in contaminated water using Tubang Bakod (Jatropha curcas L.) latex. **V.C. Badong**

228. Role of pyrrolizidine alkaloids in invasion success of *Echium plantagineum* - metabolic profiling in *Echium* spp.

D. Skoneczny, P.A. Weston, R. Callaway , L.A. Weston

229. Adsorption and desorption of methiozolin on five soils. **J. Kim**, J. Kim, J. An, S. Kim, S. Koo, K. Hwang, J. Seo*

230. Degradation of oxalic acid using Fenton oxidation processes. **Y. Kim***, H. Kwon, S. Choi, W. Oh

231. Heavy metal uptake of acacia from tailing soil in abandoned Janggun Mine, Korea. **J. Kim***, C. Lee, Y. Kim, **M. Lee**, G. Jeong

232. Remove of phenol and fluorescence dye by two-step process of titanium dioxide catalyzed photodecomposition and adsorption. **M. Cheng***, L. Au, Z. Hasan

233. Construction and improvement of microbial fuel cells using alkaliphiles.

S. Ebe*, T. Ohike, M. Okanami, T. Aono

234. Studies on metals and speciation of metals in rice. **J. Sneddon***

235. Production of a β -1,3-glucan hollow fiber due to an environmental stress response in plant protoplasts. **S. Tagawa**, Y. Yamagishi, U. Watanabe, R. Funada, T. Kondo*

236. Evaluation of lignin content in Japanese softwood species by pyrolysis-gas chromatography/mass spectrometry. **H. Yoshida**

237. Transport of stratospheric ozone to the free troposphere over central Chile.

R.J. Seguel*, N. Olivares, P. Sakamoto

* Principle Author

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- 238.** Effect of rubber media on the treatment of ammonia wastewater in a biological aerated filter. **P. YU**
- 239.** Preparation of butyl levulinate of cellulose using a single reaction process. **Y. Hishikawa**, M. Yamaguchi, S. Kubo, T. Yamada*
- 240.** Development of TiO₂ nanotube layer anodized in EG electrolyte for environmental decontamination. **S. Oh**, J. Jang*
- 241.** Indirect radiocarbon dating using microscope observation and bibliographical consideration of calligraphy. **H. Oda***, H. Yasu, S. Sakamoto, K. Ikeda

Wednesday Afternoon

Hilton Waikiki Beach
Prince Edward

Ferrites and Ferrates: Chemistry and Applications in Sustainable Energy and Environmental Remediation (#13)

Organized by: V. Sharma, R. Doong, H. Kim

- 13:00** Introduction
- 13:05 – 242.** Participation of multi-oxidants in the pH dependence of the reactivity of ferrate(VI). **K. Yoshizawa***
- 13:40 – 243.** DFT study on the oxidation of sulfite and arsenite by ferrate. **C. Chuang***, G. Liu*, M. Sung*
- 14:15 – 244.** Encapsulation of ferrate for air purification application. **R. Wu**, E. Kanchanatip, **W. Den**
- 14:40** Break
- 14:55 – 245.** Removal of tetrabromobisphenol A by ferrate(VI)-ozone oxidation technology: degradation, bromate inhibition, and toxicity evaluation. **W. Dong***, Q. Han*, H. Wang*, F. Sun*, Y. Tian*
- 15:20 – 246.** Effect of ferrate(VI) and UV radiation on THMs formation. **C. Li***, J. Zhao
- 15:45 – 247.** Comparison of the effect of ferrate and ozone pre-oxidation on disinfection byproduct formation. **Y. Jiang***, J. Goodwill, D. Reckhow, J. Tobiason
- 16:10 – 248.** Preliminary study of oxidation of selected aliphatic amino acids and dipeptides by Ferrate (VI). **L. Chen**, V. Sharma
- 16:35 – 249.** Use of chemical and biological characterization to evaluate the toxicity of drinking water disinfection by-products following chloramination, chlorination, or a novel ferrate disinfection process. **L. Cizmas***, C. Gray, V. Sharma, L. Chen

Hilton Waikiki Beach
Prince David

NanoInterfaces and their Role in Environmental Systems and Processes (#86)

Organized by: D. Dionysiou, J. Gardea-Torresdey, W. Lee, X. Zhao, B. Pan, M. Litter
Presiding: B. Pan

- 13:00 – 250.** Removal of arsenic and metals from water using nano-adsorbents. **H.J. Shipley**, D. Wagle, K. Engates, J. Hu, V. Grover
- 13:30 – 251.** Chemical hardness in the adsorption of oxoanionic species onto metal oxide nanoparticles. **Y. Suh***, F. Belay, K. Cho*
- 14:00 – 252.** Unique phosphate uptake behavior of lanthanum hydroxides nano-clusters confined in polymeric network. **Y. Zhang**, B. Pan*, X. Gao
- 14:30** Break
- 14:45 – 253.** Effect of aging method on adsorption and elution of phosphate and crystallite size in Mg/Fe layered double hydroxide. **M. Kurashina***, Y. Ogawa, E. Kanezaki
- 15:15 – 254.** Characterization of co-sorption of tungstate and cobalt on boehmite (γ -AlOOH): Uptake mechanisms of the sorption. **H. Hur**, R.J. Reeder, S. Lee, **Y. Lee***
- 15:45 – 255.** Adsorption of chlorophenols from aqueous solutions by single-walled carbon nanotubes. **H. Ding**, X. Li, J. Wang, **C. Chen***, X. Zhang

Hilton Waikiki Beach
Territorial III

Chemistry and Biology of Auxin, Strigolactone and their Interactions (#107)

Organized by: T. Asami, Y. Zhao, C. Beveridge
Presiding: S. Al-Babili, T. Asami

- 13:00** Lunch Time
- 13:30 – 256.** Current view of the auxin biosynthesis and inactivation pathways in plants. **H. Kasahara***
- 14:00 – 257.** Molecular mechanisms of auxin biosynthesis. **Y. Zhao***
- 14:30 – 258.** Local auxin metabolism in hypocotyl plays crucial roles in modulating environment-triggered rapid hypocotyl elongation. **J. chory**, z. zheng*
- 15:00 – 259.** Roles of auxin and strigolactones in the control of rice tillering. **D. Sang**, L. Jiang, D. Chen, X. Liu, N. Zhang, Q. Qian, J. Li, **Y. Wang***
- 15:30** Coffee Break

- 15:50 – 260.** Novel chemical tools for auxin biology ~auxin-biosynthesis inhibitors. **Y. Shimada**, Y. Kakei, A. Nakamura, R. Kikuchi, K. Soeno
- 16:20 – 261.** New auxin analogs that selectively modulate auxin transport via PIN localization. **K. Hayashi***, A. Ochi, H. Motose, K. Takahashi, T. Kinoshita, H. Nozaki

Hilton Waikiki Beach
Kauai

UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204)

Organized by: G. Knight, W. Liu, K. Bell, M. Mohseni, K. Linden, G. Shin, K. Oguma
Presiding: W. Liu, M. Mohseni

- 13:00 – 262.** DBPs formed from chlorine following the LP-UV and MP-UV irradiation of the ammonia containing raw water. **W. Liu***, X. Gao, X. Nie, Z. Ye
- 13:30 – 263.** Understanding the UV disinfection of wastewater: The role of influent quality and process parameters. **R. Farhood***
- 14:00** Wednesday PM Break
- 14:10 – 264.** Chlorine/UV for selective degradation of micropollutant. **E.R. Blatchley***
- 14:40 – 265.** Vacuum UV (VUV) based advanced oxidation: Scale up considerations and field evaluation. **M. Mohseni**
- 15:10 – 266.** Prediction of organic micropollutant elimination during treatment of municipal wastewater effluent with UV/H₂O₂. **Y. Lee***, U. von Gunten

- 15:40 – 267.** Comparison of UV and ozone based advanced oxidation processes for oxidation of micropollutants. **M. Kwon***, Y. Jung, H. Kae, H. Oh, T. Hwang, J. Kang*
- 16:00 – 268.** Modeling of UV fluence rate in an annular reactor for advanced oxidation of trace organic contaminants: Significance of reflection. **T. Zhang**, L. Cheng, R.G. Arnold, S. Snyder, E. Saez
- 16:20 – 269.** Understanding and predicting fate of degradation of organic compounds and associated transformation products in aqueous-phase UV photolysis and UV/H₂O₂ advanced oxidation process. **D. Minakata**, D. Kamath, S. Mezyk
- 16:40 – 270.** Applications of ceramic membrane filtration and UV oxidation synergism. **J. Alvey**

Hilton Waikiki Beach
Hawaii

Environment and Gene Interaction (#336)

Organized by: G. Cobb, C. Matson, M. Hecker, C. Wong
Presiding: C. Matson

- 13:00 – 271.** Altered reproductive capacity of Japanese medaka exposed to maternally transferred TBCO. **D. Saunders**, J. Sun, h. peng, J.P. Giesy, S. Wiseman
- 13:30 – 272.** Effects of short term and multi-generational exposures to PAHs in fishes: Laboratory and field studies. **R.T. Di Giulio***

- 14:00 – 273.** Evolutionary toxicology: Gradient of heritable resistance to PCBs and PAHs in Gulf killifish (*Fundulus grandis*) from Galveston Bay, Texas, USA. **C. Matson***, E. Ozilov, B. Dubansky
- 14:30** Break
- 14:45 – 274.** Quantification of antibiotic resistant bacteria and genes in urban watersheds. **J. He**, A. Low
- 15:15 – 275.** Natural role of polytoxin: Really a toxin or a modulator of microbial communities? **T. Yamazaki***, Y. Taira, S. Yang, H. Izumi, S. Aratake, J.D. Reimer, H. Jenke-Kodama
- 15:45 – 276.** Atmospheric emissions of veterinary pharmaceuticals from CAFOs. **G. Cobb**, B. Blackwell, P. Smith

- 16:15** Closing and Summary

Hilton Waikiki Beach
Prince Johah

Fukushima and Radiological Contaminated Environments World-wide: The Important Role of Environmental Chemistry and Radiochemistry in Remediation and Restoration (#374)

Organized by: T. Sasaki, H. Nitsche, C. Liu, Z. Yoshida, S. Kalmykov, L. Rao
Presiding: K. Iijima, C. LIU, T. Ohnuki, L. Rao

- 13:00 – 277.** Lessons we have learned from radiological accidents: The behavior of Cs-137 in the environment. **S.B. Clark***
- 13:40 – 278.** Radionuclides sorption and migration characters in the candidate land fill site. **L. Du**, Z. Tan, **X. WANG***
- 14:05 – 279.** Actinide transport in the vadose zone: Observations from old and new field lysimeter studies. **B.A. Powell***, D.I. Kaplan, L. Bagwell, H. Emerson, K. Roberts, M. Witmer
- 14:30** Break
- 14:40 – 280.** Insights into the future of radionuclide retention in Fukushima soils from first principles simulations. **K. Rosso***, M. Sassi, M. Okumura, S. Kerisit, M. Machida

- 15:05 – 281.** Physicochemical characterizations of radioactive particles emitted at the Fukushima Dai-ichi Nuclear Power Plant accident. **Y. Satou**, K. Adachi, T. Ono, Y. Iizawa, Y. Abe, I. Nakai, Y. Igarashi, K. Sasa, K. Sueki
- 15:30** Break
- 15:40 – 282.** Radionuclides sorption on soil: Surface complexation model and its application. **W. Wu**
- 16:05 – 283.** Pu transport mechanisms in the environment: Field evidence, conceptual models, and experimental data. **m. zavarin***

- 16:30 – 284.** Radionuclides removal by graphene oxide. **S.N. Kalmykov**, A.Y. Romanchuk, A. Slesarev, J. Tour
- 16:55** Closing remarks

Hilton Waikiki Beach
Molokai

Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400)

Organized by: M. Tunick, L. Liu, X. Liao, H. Nabetani, S. Yoon, X. Dai
Presiding: L. Liu, M. Tunick

- 13:00** Introductory Remarks
- 13:05 – 285.** Production of bioactive lipids, conjugated linoleic acids, using hydrogenation process. **S. Yoon***
- 13:35 – 286.** Optimal parameters to produce microencapsulated Kenaf seed oil (MKSO) by co-extrusion technology. **K. Nyam***

- 14:05 – 287.** Manipulation of molecular design of vegetable oil-based polymers for high performance. **J. Zhang***
- 14:35 – 288.** Biobased products via microwave-assisted malation of tung oil. **Z. Liu***, C. Liu, B. Tisserat, R. Wang, T.P. Schuman, Y. Zhou, L. Hu

- 15:05** Break
- 15:20 – 289.** Alternative uses for important U.S. agro-industrial coproducts. **A. Sousa**, N. Nghiem, P.M. Tomasula, L. Liu

- 15:45 – 290.** Stimulation of sulforaphane production in broccoli under modified atmosphere. **Y. Makino***, Y. Nishimura, S. Oshita, T. Akihiro, T. Mozosoe
- 16:10 – 291.** Evidence for the multifunctional bioactive properties of hemp seed peptides during oral administration to spontaneously hypertensive rats. **R. Aluko***
- 16:35 – 292.** Preparation of Si/V₂O₅ film for low moisture barriers. **H. Chiu***, C. Huang, Y. Liao*, S. Chong

Wednesday Evening

Hawaii Convention Center
Halls I, II, III

Ferrites and Ferrates: Chemistry and Applications in Sustainable Energy and Environmental Remediation (#13)

Organized by: V. Sharma, R. Doong, H. Kim

Poster Session

19:00 – 21:00

- 293.** Ferrate prepared through microwave-assisted wet oxidation method and its decoloring performance towards eosin Y. **X. Chen**
- 294.** Degradation of 2,6-dichlorophenol by liquid ferrate(VI). **B. Gwak**, I. Kim
- 295.** Degradation of 2,4-dichlorophenol using ferrate(VI) synthesized by wet oxidation method. **K. Park***, I. Kim

Hawaii Convention Center
Halls I, II, III

NanoInterfaces and their Role in Environmental Systems and Processes (#86)

Organized by: D. Dionysiou, J. Gardea-Torresdey, W. Lee, X. Zhao, B. Pan, M. Litter
Presiding: D. Dionysiou

Poster Session

19:00 – 21:00

- 296.** Enhanced stability of natural dye incorporated in mesoporous silicate. **Y. Kohno**, Y. Maeda
- 297.** Mechanism elucidation of direct adhesions between polyimide films and stainless steel substrates. **H. Akabori**, K. Iijima, M. Hashizume
- 298.** Immobilization of metal oxide nanostructures on the surface of cellulose fibers of paper matrices and study of the photocatalytic and antibacterial activities. I. Chauhan, S. Aggrawal, P. Mohanty*
- 299.** Superhydrophobic hollow silica microspheres for highly efficient recyclable smart materials for oil/water separation. M. Islam, W. Choi, H. Jeon, Y. Jin, H. Lee*

* Principle Author

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- 300.** Immobilization of poly(acrylic acid) on poly(tetrafluoroethylene) substrate surfaces for biomedical applications using supercritical carbon dioxide treatments. **A. Furukawa***, K. Iijima, K. Otake, M. Hashizume
301. Enhanced reactivity of Bi/Fe⁰ by trace amount of citric acid in degradation of chlorophenols. **J. Gong**, Y. Chang, Y. Chang*
302. Removal of heavy metals from aqueous solutions using biogenic magnetite nanoparticles. **Y. Kim***, Y. Roh

Hawaii Convention Center
Halls I, II, III

Sustainable Chemistry: Beyond the Bench (#103)

- Organized by:* M. Abraham, M. Gonzalez, P. Jessop, M. Hearn
Presiding: M. Abraham
Poster Session
19:00 – 21:00
- 303.** Catalyst development for green oxidation chemistry. **C.J. Davy***, T.J. Collins, L.J. Wright
304. Simultaneous production of vitamin E and biodiesel from waste oils obtained during edible oil refining. **K. Hiromori**, S. Borjigin, N. Shibasaki-Kitakawa*
305. Immobilized iron TAML oxidation catalysts for drinking water purification. **N. Ismail**, T.J. Collins, L.J. Wright
306. Catalytic oxidation of organic compounds by macrocyclic tetraamide complexes. **X. Lin***, T.J. Collins, L.J. Wright
307. Green processing technologies for the valorization of waste mussel shells. **J.N. Murphy**, K. Hawboldt, F. Kerton*

Hawaii Convention Center
Halls I, II, III

Chemistry and Biology of Auxin, Strigolactone and their Interactions (#107)

- Organized by:* T. Asami, Y. Zhao, C. Beveridge
Poster Session
19:00 – 21:00
- 308.** Hormonal diterpenoids besides gibberellin are involved in photomorphogenesis of *Physcomitrella patens*. **S. Miyazaki**, S. Park, H. Kawade, K. Hayashi, T. Asami, M. Nakajima*
309. Screening of chemicals that affect protonemal differentiation of *Physcomitrella patens*. **M. Nakajima***, C. Yang, S. Miyazaki, S. Park, M. Otani, H. Kawade, K. Hayashi, T. Asami
310. Auxin biosynthesis inhibitor effectively targets YUCCA. **Y. Kakei***, C. Yamazaki, M. Suzuki, A. Nakamura, A. Sato, Y. Ishida, R. Kikuchi, S. Higashi, Y. Yamasaki-Kokudo, T. Ishii, K. Soeno, Y. Shimada

Hilton Waikiki Beach
Kauai

UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204)

- Organized by:* G. Knight, W. Liu, K. Bell, M. Mohseni, K. Linden, G. Shin, K. Oguma
Presiding: M. Mohseni
19:00 – 311. Development of a simulator for design and optimization of advanced oxidation reactors. **F. Taghipour***
19:30 – 312. UV/chlorine as an alternative to UV/H₂O₂ for advanced oxidation treatment of drinking water. **R. Hofmann***
20:00 – 313. Kinetics modeling and performance assessment of UV advanced oxidation processes on trace organics removal in complex water matrices. **H. Liu***, L. Li

- 20:20 – 314.** Phototransformation of iodinated contrast media and implication in the formation of iodinated disinfection by products. **S. Allard***, C. Falantin, J. criquet, J. Croue
20:40 – 315. Pilot study using engineered photolysis for the photolytic degradation of landfill leachate. **P. Thimmaraju***, S. Bolyard, D. Reinhart, D. Soulsby, B. Cottrell

Hawaii Convention Center
Halls I, II, III

Food Processing: Chemistry, Quality, Safety, Sustainability, and Value-added By-products (#400)

- Organized by:* M. Tunick, L. Liu, X. Liao, H. Nabetani, S. Yoon, X. Dai
Presiding: L. Liu, M. Tunick
Poster Session
19:00 – 21:00
- 316.** Fabrications of pullulan and pectin submicron fibers by electrospinning. **L. Liu***
317. Improving the functionality of *Citrus junos* Tanaka (yuzu) juice by underwater shock wave pretreatment. **E. Kuraya***, S. Nakada, O. Higa, S. Itoh
318. Enhancement of anti-wrinkle activities of *Agastache rugosa* by lactic acid fermentation. **H.Y. Lee***, N. Kim
319. Adsorption of Shiga toxin to foods containing indigestible components. **K. Yokogawa***, M. Tsuji, T. Goto
320. Alaska pollock fish oil as nutritional and functional ingredient for processed muscle foods. **A. Hunt***, R. Draves, J.W. Park
321. Injection of marinade made of fish protein and nano fish bone for improved nutrition and eating quality of frozen fish fillets. **J.W. Park**, A. Hunt
322. Analysis of deterioration in early stage of frying oil. **M. Kiuchi***, M. Maki, M. Iwamatsu, M. Kataoka
323. CO₂ processing of fruit and vegetable tissues by CO₂ clathrate hydrate formation. **S. Takeya***, K. Nakano, M. bat, H. Umeda, A. Yoneyama, K. Hyodo, T. Takeda, S. Matsuo
324. High levels of icosapentenoic and docosahexaenoic acid in the lipid of the Humboldt squid, *Dosidicus gigas*: A healthful marine food. **h. saito***
325. Nitrosation reaction of amines under freezing condition. **K. Kitada**
326. DNA protection and antioxidant potential of chestnut shell extracts. **J. Lee**, K. Seo, y. Lee, T.K. Park, B. Lim
327. Validation of quantification method for ethyl carbamate in four food matrices. **B. Choi**, D. Ryu, E. Kim, S. Park, H. Paeng, E. Koh*

- 328.** Effects of temperature and period of fermentation on total phenolics and antioxidant activity of Maesil (*Prunus mume*) extract. **B. Choi***, E. Koh
329. Effect of predehydration for freezing of walleye pollock roes. **Y. Uchiiumi***, T. Suzuki
330. Title comparison of ice structure formed in homogenous or inhomogeneous food martials by freezing under conditions of deep supercooling. **R. Kobayashi***, T. Suzuki
331. Study on freezing induced texture softening of fish meat considering collagen degradation. **T. Kobayashi***, M. Watanabe, T. Suzuki
332. Oxidative stability of pork meat sausage: Effect of bee pollen extract as natural antioxidant. **S.T. Carpes**, M. Blanchin, J.d. Almeida, H.H. Carlin de Lima, A.S. Reis, D. Pereira, I.S. Ribeiro, M.S. Oviedo, C.W. Haminiuk, C. Moura
333. Functional properties, antioxidant capacity, and sweetener potential during drying process of Stevia rebaudiana leaves. **R.A. Lemus-Mondaca***, L. Zura, A. Vega, P. Rojas
334. Decomposition inhibition of the perishable food using a visible-light-active TiO₂ photocatalyst without cooling. **K. Satahira**, K. Nakasone, T. Ihara*

Hilton Waikiki Beach
Hawaii

Chemicals of Emerging Environmental Concern: A Global Perspective (#19)

- Organized by:* G. Cobb, J. Giesy, M. Murphy
Presiding: G. Cobb
8:00 Welcome and Introduction
8:05 – 351. Lessons learned from pharmaceuticals to understand bioaccumulation of ionizable environmental contaminants. **B.W. Brooks**
8:35 – 352. Untargeted screening of brominated compounds in sediments using a data independent precursor isolation and characteristic fragment (DPIC-Frag) method. **J.P. Giesy***, h. peng, c. chen, D. Saunders, S. Tang, G.P. Cooling, M. Hecker, S. Wiseman, P.D. Jones, A. Li, N. Sturchio, K.J. Rockne

- 335.** Use of reducing/nonreducing two-dimensional electrophoresis for study of disulfide-mediated interactions among proteins in egg white during storage. **S. Ishikawa***

- 336.** Development of low-allergenic prawn protein using polysaccharide as a substrate for Maillard reaction. **T. Komoda***, N. Sasaki

- 337.** Fate of dimethachlor during tobacco planting and processing. **L. Chen***, H. Cui, F. Yu, L. Pan, L. Zhao, H. Liu

- 338.** Preparation of cross-linked β -glucosidase aggregates for synthesis of salidroside, a nutraceutical additive. **X. Shi**, L. He, Y. Xue

- 339.** Development of carrot (*Daucus carota* L.) juice powder using spray drying by response surface methodology and perturbation plot. Q. Chen, J. Bi, R. Chen, X. Liu, X. Wu, J. Yi, L. Zhou, M. Zhou

- 340.** Influence of explosion puffing drying conditions on physicochemical properties of blueberries. **J. Bi**, Q. Chen, X. Wu, C. Shao, X. Liu, X. Si

- 341.** Inhibition and criterion of deterioration of frying oil by titanium oxide plate. **K. Munakata**, I. Aruse, N. Koseki, S. Eguchi, A. Sasaki, M. Endo

- 342.** Phenolic profiles and antioxidant activity of different fractions in whole brown rice. **H. Ti***, M. Zhang*, R. Zhang*, Y. Zhang, Z. Wei, Y. Deng, L. Liu, X. Tang, Y. Ma

Thursday Morning

Hilton Waikiki Beach
Prince Edward

Ferrites and Ferrates: Chemistry and Applications in Sustainable Energy and Environmental Remediation (#13)

- Organized by:* V. Sharma, R. Doong, H. Kim

- 8:00 Break**

- 8:05 – 343.** Potassium ferrate(vi) performance in the removal of selected micropollutants. **J. Jiang***

- 8:40 – 344.** Transformation of olefins and thiethers by aqueous ferrate(vi): Implications for organic micropollutant elimination during water treatment with ferrate(vi). **Y. Lee***

- 9:15 – 345.** Ferrate-induced iron particles during ferrate(vi) treatment of secondary effluent. **Y. Deng**

- 9:40 Introduction**

- 9:55 – 346.** Electrochemical ferrate(vi) synthesis by using sponge iron. **X. Sun***

- 10:20 – 347.** Kinetic investigations of the oxidation of p-chlorophenol by ferrate(vi). **z. luo**

- 10:45 – 348.** Rapid and efficient degradation of dimethylphthalate by ferrate/titanium dioxide composites. **S. Yang, R. Doong***

- 11:10 – 349.** Sequential treatment of mining waste using bacterial assisted fuel cell technology. **W. Ju**, E. Jho, K. Nam

- 11:35 – 350.** Recent advances made in understanding mechanisms of oxidation by ferrate(vi). **V. Sharma**, R. Zboril

Hilton Waikiki Beach
Hawaii

Chemicals of Emerging Environmental Concern: A Global Perspective (#19)

- Organized by:* G. Cobb, J. Giesy, M. Murphy

- Presiding:* G. Cobb

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- 9:05 – 353.** Occurrence of glucocorticoids and their metabolites in waters of Beijing, China. **H. Chang***, Y. Sun, D. Sun, J. Giesy

- 9:35 Break**

- 9:50 – 354.** Emerging contaminants in coastal waters: Personal care products and steroid hormones in Lyttelton Harbour, New Zealand. **S. Gaw***, P. Emmet, G. Northcott

- 10:15 – 355.** Neonicotinoids: Pollinator decline reveals also a worldwide threat on biodiversity and food production. **J. Bonmatin***, M. Chagnon, C.A. Downs, D. Goulson, C.H. Krupke, E. Long, F. Sanchez-Bayo, J.P. van der Sluis

- 10:40 – 356.** Environmental fate of synthetic growth promoters in animal agriculture: Recent progress and remaining challenges amid increasing trends in global use. **D.M. Cwiertny***, P.O. Kolodziej

- 11:05 – 357.** Biomass-based chemicals and processes with environmental concerns. **I.T. Horvath**

Hilton Waikiki Beach
Kauai

Analysis of Flavors in Specialty Asian Foods (#58)

- Organized by:* F. Chen, F. Zheng, J. Lee
Presiding: F. Chen, H. Kumagai, M. Steinhaus

- 8:00 Introductory Remarks**

- 8:05 – 358.** Characterization of the aroma-impact volatiles in some specialty Asian foods by application of the molecular sensory science approach. **M. Steinhaus***, J. Li, P. Schieberle

- 8:35 – 359.** Characterization of free and bound volatile compounds of Chinese bayberry (*Myrica Rubra*). **X. Ye***, H. Cheng

- 9:05 – 360.** Identification of predominant contributors to off-odors in thermally processed muskmelon juice. **J. Wu**

- 9:35 – 361.** Neutraceutical functions of lethionine, a flavor component from shiitake mushrooms. **H. Kumagai***

- 10:05 Session Break**

- 10:15 – 362.** Flavor changes of citrus fruits during storage are mainly determined by organic acid metabolism. **Y. Cheng**, X. Shan, L. Sheng, J. Xu, X. Deng

- 10:45 – 363.** Changes in aroma-related volatiles and genes expression during peach fruit ripening and postharvest storage. **b. zhang***, H. Liu, J. Shen, W. Xi, K. Chen*

- 11:15 – 364.** Features in citrus terpenoids production as revealed by carotenoids, limonoids, and aroma profiles of two pummelos (*Citrus maxima*) with different flesh colours. C. Liu, F. Yan, Y. Cheng, Z. Ma, X. Deng, **J. Xu***

Hawaii Convention Center
Halls I, II, III

UV Photochemistry for Water: Implications for Safe Water Disinfection and Oxidation Treatment Applications (#204)

- Organized by:* G. Knight, W. Liu, K. Bell, M. Mohseni, K. Linden, G. Shin, K. Oguma
Presiding: K. Oguma

* Principle Author

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Poster Session

10:00 – 12:00

- 365.** Inactivation and photoreactivation of *E.coli* in secondary treated wastewater by various UV light sources. **A. Ishida***, N. Kamiko
- 366.** Field test of photocatalytic solar water purifier in Thailand. **N. NEGISHI***, M. Sugasawa, C. Chawengkijwanich, N. Pimpha, S. Larpkiattaworn, J. Panichpakdee, T. Charinpanitkul, K. Kerndawee
- 367.** Enhancement of hydroxyl radical generation of aquatic using the visible light responsive photocatalysts of TiO_2 co-doped with nitrogen and vanadium. **Y. Han***, Y. Ishibashi, S. Kuwano-Nakatani, M. Takeda, T. Fukamatsu
- 368.** Development and study of process effectivity of the novel conducting polymer based photocatalysts for reactive azo dye degradation in model wastewater. **Z. Katančić***, V. Gilja, I. Peternel, Z. Hrnjak-Murgić
- 369.** Variation in dissolved component with irradiation ultraviolet light on mist of water samples. **T. Konno**, A. Sasaki, M. Endo
- 370.** Photolytic and photocatalytic degradation of microcystins: from photochemical approaches to engineering considerations. H. Zamankhan, A. Zakarsalehi, M. Eskandarian, **H. Choi***
- 371.** Photo-Fenton reaction of dissolved organic matters with Fe(III)-treated hydroxyapatite catalysts activated by adsorption of humic substances. **T. Moriguchi***, S. Nakagawa
- 372.** Application of ultraviolet irradiation to breakpoint chlorination process for ammonia removal. **A. Kubota**, N. Kamiko
- 373.** Comparative evaluation of CECs removal by UV/H₂O₂ and UV/chlorine at pilot scale plant. **T. Hwang***
- 374.** Comparison of UV-C and UV-C LED germicidal efficiency for *Marine bacillus subtilis* spore inactivation. **T. Hwang***, E. Kim, S. Nam

Hilton Waikiki Beach
Territorial III**Complex Mineral Growth and Dissolution Reactions: Collaborative Experimental and Computational Perspectives (#225)**

- Organized by:* A. Stack, J. Gale, P. Raiteri, L. Wang
Presiding: J.D. Gale, P. Raiteri, A. Stack, I. Wang
- 8:00** Opening Remarks
- 8:15 – 375.** On the pre-nucleation cluster pathway. **D. Gebauer***
- 8:55 – 376.** Computational investigation of mineral pre-nucleation speciation. **P. Raiteri***, W. Zhao, E. Byrne, R. Demichelis, M. De La Pierre, J.D. Gale
- 9:15 – 377.** Computational investigation of the crystallization of calcium oxalate. W. Zhao, **R. Demichelis***, P. Raiteri, J.D. Gale, F. Jones, N. Sharma
- 9:35 – 378.** Nucleation of metastable aragonite CaCO₃ in seawater. **W. Sun**, S. Jayaraman, W. Chen, K. Persson, G. Ceder
- 9:55 – 379.** Nucleation and growth of barium sulfate nanoparticles at organic–water interfaces. C. Dai, A. Stack, A. Koishi, A. Fernandez-Martinez, **Y. Hu***
- 10:15** Intermission
- 10:35 – 380.** In situ investigations of crystal nucleation and growth using electron microscopy in liquids. **R. Kroeger**
- 11:15 – 381.** In situ view of CaCO₃ nucleation. **J.J. De Yoreo**, M.H. Nielsen, P.J. Smets, N.A. Sommerdijk

Hilton Waikiki Beach
Prince David**Opportunities and Advancements in Rice Research and Aquaculture Research (#282)**

- Organized by:* J. Johnston, T. Arao, J. Sandahl, M. Estela, S. Beebout
Presiding: S.E. Beebout, J. Johnston, J.F. Sandahl

8:00 Opening Remarks

- 8:05 – 382.** Is arsenic in rice a public health concern? **J. Johnston***

- 8:25 – 383.** Effects of assorted cooking techniques on vitamin retention and arsenic mitigation in rice. **P.J. Gray***, T. Todorov, S. Conklin

- 8:45 – 384.** Mutagenic approaches for reducing Cd and As in rice grains. **S. Ishikawa**, M. Kuramata, T. Abe, T. Arao

- 9:05 – 385.** Weed management techniques affect water quality and availability in rice landscapes. **S.E. Beebout***, M.A. Bunquin, J. Opena, E. Pasuquin, R. Lampayan

9:25 Break**9:40** Remarks

- 9:45 – 386.** Mineral extracts used as feed additive to control pathogens and stimulate immune system on shrimps *Litopenaeus vannamei*. **C.T. Le***, M. Arella, G. Lafreniere Di Fruscia, F. Ascencio-Valle, H. Villarreal-Colmenares

- 10:05 – 387.** Antimicrobial residues in aquaculture products and what to do about it. **b. koone***

- 10:25 – 388.** Inhibition and recovery of olfactory function in chum salmon (*Oncorhynchus keta*) following copper exposure. **J.F. Sandahl***

- 10:50 – 389.** Effects of pesticides on fish and rice culture. **M. Islam***

- 11:10 – 390.** Current status of pesticide usage and its elimination in rice-cum-fish system in the mekong delta, Vietnam. **P.T. Nguyen***

11:30 Concluding RemarksHilton Waikiki Beach
Prince Johah**Advances in Functional Foods and Flavor Chemistry Research (#329)**

- Organized by:* M. Qian, Z. Chen, M. Herderich, C. Wang, H. Tamura, K. Wilkinson, A. Mitchell, Q. Li
Presiding: M. Herderich, M. Qian

8:00 Introduction

- 8:05 – 391.** Multidimensional and chiral studies for flavour analysis and assessment. **P.J. Marriott***, S. Chin, M. Capobianco, Y. Wong

- 8:25 – 392.** Simple HPLC-MS/MS approach to the analysis of potent thiols at ultra-trace levels in wine. **D.W. Jeffery***, R. Ristic, K.H. Pardon, D.L. Capone

- 8:45 – 393.** Development of a method for purification of thiols. K. Sakaguchi*, D. Sugimoto, H. Kasuga, **Y. Taguchi**

- 9:05 – 394.** Application of sorptive bar solid extraction for the analysis of flavor compounds in Tequila spirits. **P.A. VAZQUEZ-LANDAVERDE***

9:25 Break

- 9:40 – 395.** Defining the grape metabolome and its relationship with wine composition through comprehensive HPLC-MS/MS profiling of non-volatile grape and wine compounds. **M. Herderich***,

- N. Lloyd, V. Hysenaj, M. Solomon, M. Parker, J. Hack, D. Perzoneni, F. Mattivi

- 10:00 – 396.** Tannins structural characterization by quantitative ³¹P-NMR analysis: An unprecedented tool for tannins analysis, screening, and quality control. **C. Crestini***, H. Lange

- 10:20 – 397.** Characterization of butter aroma in terms of solvent extraction and Lod method. **H. Tamura***, S. Ueno, A. Naka, H. Zhao, Q. Chen, L. Yonekura, R. Yang, T. Isogai, R. Wakui, M. Shiota

- 10:40 – 398.** Recent advances in gas chromatography retention model and retention mechanism. **L. Wu**, Q.X. Li
11:00 Closing remark

Hilton Waikiki Beach
Molokai**Status and Trends of Persistent Organic Chemicals in the Environment (#402)**

- Organized by:* L. Bommanna, S. Masunaga, P. Kodavanti, J. Khim
Presiding: L. Bommanna, J. Khim

8:00 Introductory Remarks

- 8:10 – 399.** Spatial and temporal trends of persistent organic chemicals with emphasis on brominated flame retardants. **P. Kodavanti***, L. Bommanna

- 8:40 – 400.** Contamination of water bodies by persistent organochlorine and organophosphate pesticides in cotton cropping area. **T. Jindal**, S. Thakur, K. Gulati, A. Kumar, A. Ranjan, R. Lal, P. Jain

- 9:10 – 401.** Fluorinated alkyl acids in captive dolphins and their diet from Hawaii. **J.L. Reiner***, H. Horton, C. Bryan

- 9:30 – 402.** Effect-directed assessment of AhR-active PAHs in oil-contaminated sediments by the Hebei Spirit oil spill, South Korea. **S. Hong**, S. Jeon, B. Kwon, U. Yim, W. Shim, J. Giesy, J. Khim*

- 9:50 – 403.** Lessons learned from 15 years of monitoring contaminants in Pacific seabird eggs. **S.S. Vander Pol***, P. Becker, C.E. Bryan, R. Pugh, D.G. Roseneau

10:10 Break

- 10:30 – 404.** Spatial and temporal trends of persistent organic pollutants in ringed seals from the Canadian Arctic. **D. Muir**, X. Wang, E. Barresi, E. Sverko, S. Ferguson, B. Young

- 11:00 – 405.** Persistent toxic substances in estuarine and coastal areas of the Yellow Sea regions: An international perspective. **J. Khim***, S. Hong, B. Kwon, T. Wang, Y. Lu, J. Giesy

- 11:20 – 406.** Continuous monitoring of polychlorinated dibenz-p-dioxins and dibenzofurans in the air collected from the background area in China:2007-2014. **M. Zheng**, L. Gao, Q. Zhu, Q. Fu, Y. Lv

- 11:40 – 407.** Spatial and temporal distributions of POPs and PAHs in sediment from Masan Bay, Korea. **H. Lee***, X. Jin, S. Lee, A. Shen, Y. Jeong, S. Lee, H. Moon

Thursday AfternoonHilton Waikiki Beach
Prince Edward**Ferrites and Ferrates: Chemistry and Applications in Sustainable Energy and Environmental Remediation (#13)**

- Organized by:* V. Sharma, R. Doong, H. Kim

13:00 Introduction

- 13:05 – 408.** Sustainably sound strategies for the production of nanometal-adorned ferrites and their safer applications in catalysis and remediation. **R.S. Varma**

- 13:40 – 409.** Synthesis of monodisperse ferrite nanocrystals and $M\text{-Fe}_2\text{O}_4$ heterostructures for effective degradation of nitrophenols. **F. Lin**, **R. Doong***

- 14:15 – 410.** Catalytic ozonation of sulfamethoxazole by magnetic mesoporous molecular sieve. **C. Chang**, H. Kuo

14:40 Break

- 14:55 – 411.** Generation of OH radical in the treatment of dye effluent by zero-valent iron (ZVI). **T. Harada***, Y. Kawai

- 15:20 – 412.** Carboxymethyl chitosan functionalized magnetic core dendrimers for environmental applications. **H. Kim**, J. Park*

- 15:45 – 413.** Experimental determination of storage solution and regenerants of magnetic-cored dendrimers. **K. Kim**, H. Kim, J. Park*

- 16:10 – 414.** Investigation of reducing capacities and redox potentials of sewage sludge humic substances with iron oxides. **J. Jiang***, Z. Yang

- 16:35 – 415.** Degradation of BTEX in aqueous solutions using Fe_3O_4 activated per-sulfate oxidation system. **C. Hung**, C. Chen, Y. Liu, **C. Dong**

Hilton Waikiki Beach
Hawaii**Chemicals of Emerging Environmental Concern: A Global Perspective (#19)**

- Organized by:* G. Cobb, J. Giesy, M. Murphy
Presiding: J.P. Giesy

13:00 afternoon introduction

- 13:05 – 416.** Applications of environmental forensics for chemicals of emerging concern. **K.J. Rockne**, G.P. Codling, J.P. Giesy

- 13:30 – 417.** Occurrence of PPCPs in Chinese streams: A nationwide study. B. Yao, S. Yan, **W. Song**

- 13:55 – 418.** PPCP/EDCs: From soil to plants. **J. Gan***, S. Wu, J. Conkle, L. Dodgen, F. Ernst

- 14:20 – 419.** Evaluating plant uptake of pharmaceuticals from soil afterment with urine-derived fertilizers. **D.S. Aga**, R. Mullen, A. Noe-Hays, K. Nace, N. Love, K.R. Wiggington

14:45 Break

- 15:00 – 420.** Chemical legacy from US military bombing. **D. Klein**

- 15:25 – 421.** Fate of emerging cyanobacterial harmful metabolites in water supply systems. **A. Zamyadi***, S. Dorner, M. Prevost, G. Newcombe, R.K. Henderson

- 15:50 – 422.** Understanding biosynthetic routes for polybrominated aromatic pollutants and toxins from the marine environment. **V. Agarwal***, B. Moore

- 16:15 – 423.** Investigation of perfluorinated alkyl substances contamination in groundwater: Influence of field sampling and laboratory analytical techniques. **D. Loock**, N. Battye, K. Reimer, K.P. Weber, I. Koch

Hilton Waikiki Beach
Kauai**Analysis of Flavors in Specialty Asian Foods (#58)**

- Organized by:* F. Chen, F. Zheng, J. Lee
Presiding: F. Chen, K. Lee, Z. Xiao, F. Zheng

13:00 Introduction Remarks

- 13:05 – 424.** Characterization of aroma compounds of Chinese famous liquors by gas chromatography-mass spectrometry and flash GC electronic-nose. **Z. Xiao**

- 13:35 – 425.** Chemical profiles and antioxidant activity of volatile extracts isolated from Korean rice beers and wines. **K. Lee**

- 14:05 – 426.** Analysis of volatiles in Chinese Dezhou braised chicken by ASE-SAFE/GC×GC-TOF MS. **F. Zheng**

- 14:35 – 427.** Chemical and sensory profiles of Korean soybean pastes using GC-olfactometry, GC-mass spectrometry, and sensory descriptive analysis. **S. Lee***

15:05 Session Breaks

- 15:15 – 428.** Differentiation of aroma compounds in Chinese bayberry by GC-MS and GC-O combined with principal component analysis (PCA). **H. Cheng***, X. Ye*

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TECHNICAL PROGRAM

15:45 – 429. Flavor component analysis of sweet potato shochu by GC-MS-based non-target analysis and sensory evaluation. **Y. Matsuo***, T. Namiki, K. Toyama, S. Oda, K. Yamazaki, T. Nakajima
16:15 – 430. Investigation of the sunlight-induced aroma deterioration of pummelo (*Citrus maxima*) essential oil. **H. Ni***, P. Hong, H. Sun, F. Chen, H. Cai

Hilton Waikiki Beach
Territorial I & II

Advanced Products from Lignin and Micro- or Nano-fibrillated Cellulose (#70)

Organized by: T. Hu, A. Ragauskas,
H. Hatakeyama
Presiding: T. Hu

13:00 – 431. Overcoming challenges on the development of nanocellulose-based products. **M. Peresin***, T. Hänninen, M. Hakalahti, J. Pere, V. Kunnari, J. Varianen, P. Qvintus, T. Tamminen
13:25 – 432. Commercial advances in the application of fibrillated cellulose. **A. Dodd***, S. Winter

13:50 – 433. Effect of micro- and nanofibrillated celluloses on the structure, physical properties, and dewatering of a composite paper. **J.J. Rantanen***, T. Maloney

14:15 – 434. Nanocellulose composites: Optimization of properties and process. **P. Raj***, S. Varanasi, W. Batchelor, G. Garner

14:40 – 435. Effect of cellulose nanofibrils on curing behaviour of epoxy amine systems. **N. Yan**

15:05 Break

15:15 – 436. Nanofibrillation of dried pulp in NaOH solutions and applications. **K. Abe***, H. YANO

15:40 – 437. Cellulose nanopaper with controllable optical properties. **M. Hsieh***, H. Koga, M. Nogi, K. Suganuma

16:05 – 438. Xylan tyramine conjugate as a biomimetic crosslinker for 3D bioprinted materials from trees. K. Markstedt, G. Toriz, **P. Gatenholm**

Hilton Waikiki Beach
Territorial III

Complex Mineral Growth and Dissolution Reactions: Collaborative Experimental and Computational Perspectives (#225)

Organized by: A. Stack, J. Gale, P. Raiteri, L. Wang
Presiding: J.D. Gale, P. Raiteri, A. Stack, I. wang

13:00 – 439. In situ scanning transmission X-ray microscopic analysis of biofilm formation and dissolution of sulfide minerals by *Acidithiobacillus ferrooxidans*. **S. Harmer***

13:20 – 440. Fe(II)-catalyzed recrystallization of hematite and goethite: Experimental observations, computational questions. **M. Scherer***, K. Rosso, D.E. Latta, A. Friedrich, M. Helgeson

13:40 – 441. Iron electron transfer, atom exchange, and Fe oxide growth at the clay mineral-water interface. **D.E. Latta***, W. Premaratne, K. Rosso, M. Scherer, A. Neumann

14:00 – 442. Molecular-scale change of the hydration structure of calcite surfaces due to magnesium ions probed by FM-AFM. **Y. Araki**, H. Onishi, N. Oyabu, K. Kobayashi, H. Yamada

14:20 – 443. Combined experimental and computational analysis of silica-water interfaces to understand dissolution mechanisms. **J.D. Kubicki***, J. Boettger, M. DelloStritto, J. Sofo, M. Fedkin, A. van Duin, D. Wesolowski, P. Fenter, S. Gomez, F.M. Geiger

14:40 – 444. Reactive surface area in the environment: New solid-state NMR tools coupled with computational chemistry. **K.T. Mueller***, N. Washiton

15:00 Intermission

15:20 – 445. Monte Carlo simulation of nanoporous crystal growth. **M.W. Anderson***, J.T. Gebbie

15:40 – 446. Atoms to pores growth of barite. **A. Stack**
16:00 – 447. Fingerprint patterns induced by precipitation reactions during injection in porous media. **A. De Wit***, G. Schuszter, F. Haudin, P. Shukla, F. Brau, J. Cartwright, Y. Nagatsu
16:20 Closing remarks/Open Discussion

Hilton Waikiki Beach
Prince Johah

Advances in Functional Foods and Flavor Chemistry Research (#329)

Organized by: M. Qian, Z. Chen, M. Herderich, C. Wang, H. Tamura, K. Wilkinson, A. Mitchell, Q. Li
Presiding: H. Tamura, K. Wilkinson

13:00 Opening remark: Introduction

13:05 – 448. Characterization of branched long-chain aliphatic aldehyde analogs as potent odorants in ripe natural cheeses. **K. Kumazawa***, S. Inagaki, S. Fujikawa, Y. Wada

13:25 – 449. New approach to investigate the flavor release from different beverage compositions: Influence of milk on aroma release during consumption of coffee beverages. **T. Itoke**, K. Kumazawa*

13:45 – 450. Characterization of important aroma compounds in raw licorice (*Glycyrrhiza glabra*). **M. Granvogl**, J. Wagner, P. Schieberle

14:05 – 451. Formation of peppery, minty, rosy and woody sesquiterpenes derived from α -guaiene. **D. Taylor***, A. Huang, M. Sefton

14:25 – 452. Characterisation of volatile profile of Chinese rice wines by comprehensive 2D gas chromatography coupled with time-of-flight mass spectrometry (GC \times GC-TOFMS). **S. Chen***, J. Wu, N. Wang, Y. Xu*

14:45 Break

15:00 – 453. Toward a systems-based approach for hop flavoromics. **R.A. Shellie**, L. Tedone, D. Yan, L. Staskova, A. Koutoulis, S. Whittick

15:20 – 454. Combined analysis of non-targeted volatile profile and sensory evaluation of commercial tomato juices to elucidate flavor characteristics. **Y. Iijima***, Y. Iwasaki, Y. Otagiri, T. Sato, H. Otomo, Y. Sekine, A. Obata

15:40 – 455. Distinguishing the botanical origin of honey for authentication using head-space solid-phase microextraction (HS-SPME) gas chromatography mass spectrometry (GC/MS) and multivariate analysis. **A.E. Mitchell***, S. Charoenprasert

16:00 – 456. Understanding the composition of coffee quality. **H.E. Smyth***, W. Sunarhamur, H. Tran, U. Pappu, B. Cheng, J. Mayze, A. Furtado, D. Williams, S. Fuller, S. Richards, R. Henry

16:20 – 457. Impact of vineyard exposure to smoke on the composition and sensory properties of wine. L. van der Hulst, C. Ford, R. Burton, R. Ristic, N. Lloyd, Y. Hayasaka, **K. Wilkinson**

16:40 – 458. Flavor and flavor stability of ready-to-drink tea beverage during storage. F. Yuan, F. He, Y.L. Qian, J. Zheng, W. Huang, **M. Qian***

17:00 Closing remark

Hilton Waikiki Beach
Molokai

Status and Trends of Persistent Organic Chemicals in the Environment (#402)

Organized by: L. Bommanna, S. Masunaga, P. Kodavanti, J. Khim
Presiding: P. Kodavanti, S. Masunaga

13:00 – 459. Impact of crude electronic waste recycling in loading polychlorinated biphenyls in Indian environment: Implications for atmospheric outflow. **P. Chakraborty***, S. Sakthivel, P. Balasubramanian

13:30 – 460. Pilot study of the breakdown of organics present in reverse osmosis concentrate from a potable water reuse facility in a constructed wetland system.

A.K. Robinson, B. Cottrell, G. McCarthy, P. Thimmarraju, W.J. Cooper, K. Ishida

13:50 – 461. Study of analyte recovery as a function of chlorinated hydrophobic pollutant concentration and sample storage time using headspace solid-phase microextraction (HS SPME) coupled with GC-ECD. **F.M. Dunnivant***, J. Tillman, W. Weckel-Dahman

14:10 – 462. Cryo-repository and persistent organic pollutant monitoring of sea turtle tissues from the U.S. Pacific Islands region. **J.M. Lynch***, G. Balazs, C. Allen, F. Arengo, S. Benson, J. Brooker, T. Eguchi, H. Harris, B. Jensen, R. LeRoux, R.S. Pugh, M.R. Rice, J. Seminoff, E. Sterling, T.M. Summers, T. Work, P.R. Becker

14:30 – 463. Black carbon: A reactive sorbent for the destruction of persistent organic contaminants by sulfides. **W. Xu***, K. Ding

14:50 Break

15:10 – 464. Behaviors of perfluoroalkyl acid precursors in sewage treatment plants. **S. Masunaga***, F. Ye, M. Tokumura

15:40 – 465. Transformation and phytotoxicity of PBD-47 in maize (*Zea mays* L.). **S. Zhang**, S. Wang, X. Xu

16:00 – 466. Effect of addition of *Bacillus subtilis* on biodegradation of DDT by *Pleurotus ostreatus*. **A.S. Purnomo***, F.T. Hermansyah

16:20 – 467. Characteristics of PAHs adsorption on inorganic particles and activated sludge in domestic wastewater treatment. **J. Liu***

16:40 Closing remarks

Thursday Evening

Hilton Waikiki Beach
Hawaii

Chemicals of Emerging Environmental Concern: A Global Perspective (#19)

Organized by: G. Cobb, J. Giesy, M. Murphy
Presiding: G. Cobb

19:00 – 468. Aqueous organic emerging contaminants from arid, anthropogenic watersheds of North America. **L. Abrell***, C. Carreón-Díazcontí, I. Avifla-Lamarque, R. Preciado-Monjardin, M. Valdez-Carrillo, S. Samanthi Wickramasekara, J. Chorover

19:20 – 469. Impacts of global change on atmospheric mercury. **S. Wu**

19:40 – 470. Granulation of partial nitrifying sludge facilitated by gel carriers in treating high-strength ammonia wastewater. **Y. Li***, X. Li, R. Li, L. LIN, J. Xu

20:00 – 471. Effect of intrinsic properties of activated carbons on mercury adsorption ability. **K. Tachibana**, E. Karagianni, H. Yamaura, S. Yamaguchi, Y. Ichishima, M. Ichishima, H. Yahiro*

20:20 – 472. Experimental determination of solubilities of di-calcium ethylenedi-aminetetracetic acid [$\text{Ca}_2\text{C}_{10}\text{H}_{12}\text{N}_2\text{O}_8\text{S}$] in NaCl and MgCl₂ solutions to high ionic strengths and its Pitzer model: Applications to geological disposal of nuclear waste and other low temperature environments. **Y. Xiong***

20:40 – 473. Innovative use of carbonaceous geosorbents for sequestration of antibiotics to reduce their transport and bioavailability. **C. Liu***, Y. Chuang, Y. Zhang, H. Li, S.A. Boyd, B.J. Tepper, **W. Zhang**

Hawaii Convention Center
Halls I, II, III

Analysis of Flavors in Specialty Asian Foods (#58)

Organized by: F. Chen, F. Zheng, J. Lee
Presiding: F. Chen

Poster Session

19:00 – 21:00

474. Use of stir bar sorptive extraction and thermal desorption for gas chromatography-mass spectrometry characterization of selected volatile compounds in Chinese liquors. **Y. Niu**

475. Optimization and application of head-space-solid-phasemicro-extraction coupled with gas chromatography-mass spectrometry for the determination of volatile compounds in cherry wines. **R. Zhou**

476. Volatile compounds in foot muscle of abalone (*Halotis discus hannai* Ino) during heating process. **L. Qin***, S. Hao, H. Wang, Y. Wang, B. Zhu

477. Effect of steam cooking on physico-chemical properties of turbot (*Scophthalmus maximus* L.) muscle and its volatile compounds. **X. Dong**, Y. Wang, J. Pan, B. Zhu

478. Comparison of volatile profiles in buckwheat (*Fagopyrum esculentum*) soksgung-jang fermented with different starter combinations. **I. Cho***, M. Park, H. Choi, B. Shin, Y. Kim

479. Evaluation of Pu-erh tea by the electronic tongue: Correlation with sensory properties and chemical compositions according to different grade levels and varied ages. **L. Gao**, M. Bian, W. Zhao, X. Hu, J. Wu*

480. Regulating the functional component contents and antioxidant activity of tea leaves by fertilizing with N, P, Se, and Zn. **H. Li**

481. Comparison of volatile compounds in simulated mozzarella cheeses. **X. Wang***, L. Ma*

482. Analysis of characteristic aroma components in sesame seed oil and optimization of roasted aroma producing condition for Chinese black sesame Jinhuangma. **Y. Wan***, Y. Song, L. Bai, G. Fu, S. Nie, H. Li, M. Xie*

483. Research of volatile components in Sichuan pickles during fermentation. **B. Pu***

Hawaii Convention Center
Halls I, II, III

Complex Mineral Growth and Dissolution Reactions: Collaborative Experimental and Computational Perspectives (#225)

Organized by: A. Stack, J. Gale, P. Raiteri, L. Wang
Presiding: J.D. Gale, P. Raiteri, A. Stack, I. wang

Poster Session

19:00 – 21:00

484. Evaluating the contribution of energetically reactive surface sites to the dissolution of spent nuclear fuel analogs CeO₂ and ThO₂. **C.L. Corkhill**, D.J. Bailey, M.C. Stennett, J.A. Miller, J.L. Provis, N. Hyatt

485. Leaching behavior of radium and thorium isotopes in ishikawaite. **K. Komatsubara***, Y. Kurihara, R. Shiobara, K. Nomura, T. Nakamura, Y. Koike

486. Manipulation of the texture and elemental composition of the novel sheaths produced by the iron oxidizing bacterium *Leptothrix* in culture by altering components of the medium. **H. Kunoh***

* Principle Author

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- 487.** Formation of calcite or vaterite via reactions between gaseous CO₂ and Ca²⁺ electrolytes. G. Choi, S. Jeon, S. Namgung, J. Choi, **G. Lee***
- 488.** Leaching of radium and thorium isotopes from thorium minerals, thorite, and yttrialite. R. Shiobara*, Y. Kurihara, K. Komatsubara, T. Nakamura, Y. Koike
- 489.** Effective recovery process of insoluble Sb in urban mine by controlling the metal complexes condition in Sb-tartaric acid-OH aqueous system. **S. Ueno**, S. Yokoyama, K. Shinoda, H. Takahashi*, K. Tohji

Hawaii Convention Center
Halls I, II, III

Opportunities and Advancements in Rice Research and Aquaculture Research (#282)

- Organized by:* J. Johnston, T. Arao, J. Sandahl, M. Estela, S. Beebout
- Poster Session**
19:00 – 21:00
- 490.** Pesticide multi-residue analysis in Red Swamp crayfish using QuEChERS and HPLC/MS/MS. **L. Han**, K. Zhu, M. Feng, Z. Zhang
- 491.** Development of anode material for rechargeable battery from rice husk gasification technology. **M. Seo***, W. Cho, H. Ra, S. Yoon, Y. Kim, J. Kim, J. Lee, H. Kim, J. Choi

Hilton Waikiki Beach
Prince Johah

Advances in Functional Foods and Flavor Chemistry Research (#329)

- Organized by:* M. Qian, Z. Chen, M. Herderich, C. Wang, H. Tamura, K. Wilkinson, A. Mitchell, Q. Li
- Presiding:* M. Qian, H. Tamura
- 19:00** Opening remark
- 19:05 – 492.** Isolation, identification, and quantification of Lichenysin, a novel non-volatile compound in Chinese distilled spirits reduced the headspace concentration of phenolic off-flavors via hydrogen-bond interactions. **Y. Xu***, R. Zhang, Q. Wu

- 19:25 – 493.** Analysis and identification of characteristic aroma components in Hong Qu glutinous rice wine. **W. Zhang**, **Z. Liu**, C. Zheng, **L. Ni***
- 19:45 – 494.** Characterization of aroma compounds which induce or modulate the activity of the human sweet taste receptor. **K. Nojiri***, S. Fujiwara, T. Misaka
- 20:05 – 495.** Green synthesis of benzaldehyde from cinnamon oil. **H. Ji***
- 20:25 – 496.** Molecular characterisation of starch by NMR and FT-IR spectroscopies, and X-ray diffraction. **M. Van Leeuwen***, M. Toutounji, J. Mata, E. Gilbert, A. Shrestha, L. Pallas, R. Ward, P. Castignolles, M. Gaborieau

20:45 Closing remark

Hawaii Convention Center
Halls I, II, III

Status and Trends of Persistent Organic Chemicals in the Environment (#402)

- Organized by:* L. Bommanna, S. Masunaga, P. Kodavanti, J. Khim
- Presiding:* L. Bommanna, S. Masunaga
- Poster Session**
19:00 – 21:00
- 497.** Spatial distribution and temporal trends of polybrominated diphenyl ethers (PBDEs) in sediment and bivalves from Korean coastal waters collected between 2004 and 2013. **S. Lee***, H. Lee, X. Jin, A. Shen, J. Lee, S. Lee, Y. Jeong, H. Moon

- 498.** Source identification and seasonal variation of allochthonous organic matter in an artificial Lake Shihwa and surrounding inland creeks in South Korea. **Y. Lee**, S. Hong, J. Hur, J. Khim, K. Shin*

- 499.** Current efforts to produce environmental certified reference materials. **J. Kucklick***, J.L. Reiner, S.S. Vander Pol, K. Huncik, S. Long, S. Christopher, R. Day, J. Bowden, M. Ellisor, B. Kassim, B. Benner, A. Boggs, J. Murray
- 500.** Electrochemical process: Contribution to water environment. **D.R. Wulan***, S. Cahyaningsih, D. D
- 501.** Variations of detection of the Japanese PRTR chemicals in urban river water. **S. MIHO**, T. KAMEYA*, T. Kobayashi, K. FUJIE
- 502.** Combined instrumental and bioanalytical assessments of estuarine and coastal sediments along the west coast of Korea. **S. Jeon***, S. Hong, B. Kwon, J. Khim
- 503.** Screening and source identification of flame retardants in car indoor dust using field emission electron probe micro analyzer. **M. Tokumura***, Y. Yamatori, Y. Negishi, S. Masunaga
- 504.** Simultaneous biosorption of iodine and methanethrene by soil indigenous microorganisms. **D. Zhang***, P. Zhou, T. Lyu, H. Zhao
- 505.** Simple method for the determination of H₂S inside the shell of bivalves and its application to *Corbicula japonica*. **S. SUGAHARA***, H. KAMIYA, M. YAMAMURO, J. PARK, M. Egawa, Y. SEIKE
- 506.** Behavior of arsenic in acidic river environments. **K. Elki**, N. Sugai, A. Sasaki, M. Endo

Friday Morning

Hilton Waikiki Beach
Hawaii

Chemicals of Emerging Environmental Concern: A Global Perspective (#19)

- Organized by:* G. Cobb, J. Giesy, M. Murphy
- Presiding:* S. Gaw
- 8:00** Welcome and Introduction
- 8:05 – 507.** Detection, identification, and quantification of novel brominated flame retardants in environmental matrices. **D. Saunders***, h. peng, J. Sun, P.D. Jones, S. Wiseman, J.P. Giesy
- 8:30 – 508.** Characterization of endocrine active substances in surface waters in Taiwan using biological assays and liquid chromatography tandem mass spectrometry. **P. Chou***, K. Chen, T. Li, M. Kawanishi, T. Yagi
- 8:55 – 509.** Measurement of in vitro biotransformation rates of xenobiotic chemicals for identifying bioaccumulative organics among chemicals in commerce. **Y. Wan**, G. Zheng, J. Hu

- 9:00** Break
- 9:35 – 510.** Environmental and health issues of extensive herbicide and pesticide application from multiple agrobased activities in a tropical freshwater river system of Thailand. **B.N. Noller**, T. Komarová, C. Boonthai Iwai*, A. Somparn, N. Tokhun, J. Mueller, I.R. Kennedy
- 10:00 – 511.** Saving our bees – removing neonicotinoids from waters using oxidizing radicals. **B. Daws**, J.J. Kiddie, S. Mezyk
- 10:25 – 512.** Solvent usage for chemiluminescent labeling processes. **J.-. Grote**

- 10:50 – 513.** Mechanistic study of environmentally persistent free radical formation in phenol contaminated soils. U. Nwosu,

R. Cook*

Hilton Waikiki Beach
Territorial I & II

Advanced Products from Lignin and Micro- or Nano-fibrillated Cellulose (#70)

- Organized by:* T. Hu, A. Ragauskas, H. Hatakeyama
- Presiding:* A. Ragauskas

- 8:00 – 514.** Electrosterically stabilized nanocrystalline cellulose as a green, sustainable, advanced material. **A. Sheikhi***, T. van de Ven
- 8:25 – 515.** Chemically assembly of hydrolyzed electrosterically stabilized nanocrystalline cellulose. **H. Yang**, T. van de Ven
- 8:50 – 516.** Advances in nanolignocellulosics for foams and fills. **A. Ragauskas**, Q. Sun, T. Körnke
- 9:15 – 517.** Order of addition effects on the chemistry, structure and properties of CNC-epoxy nanocomposites. **C. Meredith***, M. Shofner, G. Schueneman, N. Giroud
- 9:40 – 518.** Technical challenges and market opportunities of nanocellulose for high volume, innovative composite-based commercial applications. **S. Ozcan***
- 10:05** Break
- 10:15 – 519.** In situ preparation of magnetic composite by immobilizing ferrite on cellulose nanocrystals. **S. Fu**, C. Tian
- 10:40 – 520.** Cellulose nanomaterials from the viewpoint of the new microfibril model. **U. Agarwal***
- 11:05 – 521.** Molecular origins of twists in cellulose materials. **K. Conley**, L. Godbout, M. Whitehead, T. van de Ven
- 11:30 – 522.** Lignin-based nanocomposite aerogels reinforced with nanocrystalline cellulose for energy storage applications. **M.A. Karaaslan**, F. Ko

Hilton Waikiki Beach
Prince Edward

Proteomics and Metabolomics in Agricultural, Environmental, and Public Health Sciences (#264)

- Organized by:* J. Johnston, Q. Li, J. Emon, J. Chen, S. Lee, C. Zhang
- Presiding:* J. Johnston, Q.X. Li, C. Zhang
- 8:00** Opening Remarks
- 8:05 – 523.** Genetic diversity of four anti-nutritional factors in kidney bean (*Phaseolus vulgaris* L.). **C. Chen**
- 8:25 – 524.** Advantage of proteomics study in microorganism involved plant-plant interaction complex. **R. Jia**, Q.X. Li, A. Guo, Y. Gu
- 8:45 – 525.** Shiga toxin-producing *Escherichia coli* analyzed by RT-qPCR, MALDI-TOF-TOF-MS/MS-PSD and top-down proteomic analysis. **C.K. Fagerquist***, W.J. Zaragoza

- 9:05 – 526.** Proteomic analysis on rice seed germination. **P. Yang***

- 9:25 – 527.** Identification and classification of rhizobia by matrix-assisted laser desorption/ionization time-of-flight mass spectrometry. **R. Jia***, Q.X. Li, Q. Wei, A. Guo, Y. Gu

- 9:45 – 528.** Workflow for SWATH-MS data processing and analysis. K.M. Frederick, N. Haverland, M. Majumder, **P. Ciborowski***

10:05 Break

- 10:20 – 529.** Identification of protein complexes and pathways contributes to *Escherichia coli* resistance to balofloxacin using native/SDS-PAGE-based proteomics. **H. Li**

- 10:40 – 530.** Expression and site-directed mutagenesis of the highly stable royal palm peroxidase in *Pichia pastoris*. **H. Zhao**, Q.X. Li

- 11:00 – 531.** Proteomics for adverse outcome pathway discovery using human kidney cells. **J. Van Emon***, F. van Breukelen , P. Pan

- 11:20 – 532.** *Stenotrophomonas* sp. L60 degrades Cry1Ab. **S. Gao**, Q.X. Li, J. Li

- 11:40 – 533.** Visualization of proteomics data for bioinformatics analyses. **K.M. Frederick**, N. Haverland, P. Ciborowski*

Hilton Waikiki Beach
Prince David

Analytical Development Relevant to Environmental Exposure and Effects (#288)

Organized by: C. Le, X. Li, G. Jiang, S. Richardson

Presiding: K. Chen, C. Le

- 8:00 – 534.** Analysis of agrichemicals in the environment using paper spray ionization mass spectrometry. S.L. Reeber, **G.L. Glish***

- 8:30 – 535.** Environmental metabolomics and ecotoxicity modeling using earthworms. **C.K. Larive***, C. Griffith

- 8:50 – 536.** Identification of flame retardant additives in consumer products using mass spectrometry and understanding human exposure pathways. **H. Stapleton***, E. Cooper, K. Davis, K. Hoffman

- 9:10 – 537.** Biomarker excretion rate as a method for assessing exposure to environmental toxicants. **B. Blount**

- 9:30 – 538.** Trace analysis of gold nanoparticles in environmental waters. **B. Hu**, B. Chen, M. He

9:50 Break

- 10:10 – 539.** Integrating analytical biology and chemistry to resolve molecular mechanisms of toxicity for water disinfection by-products. **M.J. Plewa***, J. Pals, Y. Komaki, E.D. Wagner

- 10:40 – 540.** Occurrence and toxicity of halobenzoquinones - an emerging class of disinfection byproducts in drinking water. **X. Li***, W. Wang, J. Li

- 11:00 – 541.** High resolution and tandem mass spectrometry uncovers chlorination reaction pathways for transformation of medical imaging compounds in drinking water treatment. **S. Richardson***, C. Joseph, F. Wendel, C. Luetke-Eversloh, C. Postigo, T. Terres, E. Machek, N. Ackerson, S. Duirk, E.D. Wagner, M.J. Plewa

- 11:20 – 542.** Chemical and toxicological analyses of halogenated disinfection by-products in tap water and boiled tap water. **X. Zhang***, J. Liu*, Y. Li
- 11:40 – 543.** Development of an easy and efficient tool for nitrosamine precursor concentration in water based on cation exchange. **S. Li**, E. Bei, J. Wang, **C. Chen***, X. Zhang, M. Suffet

Hilton Waikiki Beach
Prince Johah

Advances in Functional Foods and Flavor Chemistry Research (#329)

- Organized by:* M. Qian, Z. Chen, M. Herderich, C. Wang, H. Tamura, K. Wilkinson, A. Mitchell, Q. Li
- Presiding:* Q.X. Li, A.E. Mitchell

8:00 Opening remark: Introduction

- 8:05 – 544.** Trehalose bioproduction by a novel trehalose synthase from *Arthrobacter chlorophenolicus* SK38.001. **B. Jiang**

- 8:25 – 545.** Mechanisms to retain naturally-occurring anthocyanin pigments in thermally processed whole fruits in aqueous media. **Y. Zhao**, J. Jung

- 8:45 – 546.** Preparation and microstructure of food lipid nanoparticles modified by trehalose. **Z. Wen**

* Principle Author

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TECHNICAL PROGRAM

9:05 – 547. Investigation of volatile antioxidants formed from coffee beans under various roasting conditions.
T. Shibamoto*

9:25 – 548. Searching for aroma compounds which are effective for Alzheimer's disease.
K. Murata, K. Tanaka, T. Furuta, Y. Ueno, Y. Yoshioka, S. Matsumura, H. Matsuda*

9:45 Break

10:00 – 549. Anxiolytic-like effects of ylang-ylang essential oil and its major components in anxiety models in mice.

N. Zhang, L. Yao*, Y. Deng, L. Feng

10:20 – 550. Analysis and identification of bitter compounds from Lu (Solanum quitoense L.) fruit with potential ACE-inhibitory activity.
D. Forero*, C. Masatani, Y. Fujimoto, D.G. Peterson, E. Coy-Barrera, C. Osorio

10:40 – 551. Explore the physiological effect of functional foods by proteomics.
F.C. Kuo*

11:00 – 552. Carotenoid metabolism and cancer prevention.
S. Schwartz*

11:20 – 553. Procyanidins as functional food ingredients? Systemic absorption, metabolism, and bioavailability.
H. Humpf*, S. Rzeppa, K. Bittner

11:40 – 554. Heart protection of roselle drink - a human clinical trial.
C. Wang*

12:00 Closing remark

Hilton Waikiki Beach
Molokai

Radioactive Contaminants and Waste Management in the Environment (#390)

Organized by: W. Um, M. Baik,
O. Toshihiko, A. Francis, D. Kaplan
Presiding: T. Ohnuki, W. Um

8:00 – 555. Independent monitoring of the radiological release event at the Waste Isolation Pilot Plant (WIPP) repository in New Mexico, USA.
P. Thakur*

8:20 – 556. Fundamental study of conditioning of wastes generated from several contaminated water treatment devices in Fukushima Daiichi Nuclear Power Station.
Y. Meguro*, J. Sato, J. Kato, A. Nakagawa, Y. Koma, T. Ashida

8:45 – 557. Technetium and chromium release from reducing cementitious materials under laboratory and field conditions.
D.J. Kaplan*, Y. Arai, G. Flach, D. Li, B.A. Powell

9:10 – 558. Radiological contamination at US Department of Energy facilities: Lessons learned from site characterization and remediation activities.
S.B. Clark*

9:35 – 559. Uranium(VI) chemistry in natural groundwater: Chemical speciation, molecular structure, and adsorption behavior.
J. Yun*

10:00 – 560. Evaluation of fluorescence as a monitoring tool for phytoemediation of tritium.
R.L. Brigmon*, E. Doman, E. Wilde, K. McLeod, J. Seaman

10:20 – 561. Applications of two photon spectroscopy in uranium bio-geochemistry.
L. Natrajan*

10:40 – 562. Application of phytoextraction using lettuce, Chinese cabbage, and radish to the uranium contaminated soil in Korea.
M. Lee*, Y. Han, J. Kim

11:00 – 563. Geochemical behaviors of uranium in granitic groundwater.
M. Baik*, T. Park, J. Jung

11:20 – 564. Characterizing the mineralogy and redox reactivity of potential host rocks in a geological disposal facility for radioactive waste.
J. Quirke, M. Henderson, R. Patrick, K. Rosso, A. Dent, J. Sharples, C.I. Pearce*

11:40 – 565. Emerging strategies for the disposal of iodine-129 in deep geological repositories.
D. Laurencin*, L. Campayo, A. Coulon, A. Grandjean

Friday Afternoon

Hilton Waikiki Beach
Hawaii

Chemicals of Emerging Environmental Concern: A Global Perspective (#19)

Organized by: G. Cobb, J. Giesy, M. Murphy
Presiding: J. Gan

13:00 – 566. Rare earth elements as chemicals of emerging concern.
P.G. Campbell*, C. Beaubien, A. Crémazy, C. Fortin

13:25 – 567. Pollutant toxicity as measured by *Artemia Franciscana* with a focus on humic acid and surfactant interactions.
R. Williams, R. Cook

13:50 Break

14:05 – 568. Naphthenic acid property responses to environmentally relevant changes in temperature, pH, and salinity modeled with COSMO-RS solvation theory.
J.M. Parnis*, A. Celsie, D. Mackay

14:30 – 569. Utilizing chlorine atom reactivity in UV-based advanced oxidation processes: Kinetics and efficiencies of chlorine atom reactions.
K.D. Couch, T. Reuterius, S. Mezyk, K. Ishida

14:45 – 570. Chloramine dissipation models for stormwater sewers.
Q. Zhang*, E. Davies, J. Bolton, Y. Liu

15:20 Closing and Summary

Hilton Waikiki Beach
Territorial III

Pectin Chemistry and Technology (#20)

Organized by: B. Savary, M. Williams, S. Lu, S. Yoo, R. Cameron

13:00 Opening

13:10 – 571. Current models of pectin structure: How they were arrived at and how to improve them.
A.J. Mort*, X. Wu

13:50 – 572. Deciphering the structure of pectic oligosaccharides by a new tandem mass spectrometry method based on photo-activation in the vacuum ultraviolet range.
D. Ropartz*, A. Giuliani, J. Lemoine, P. Dugourd, **M. Ralet**, H. Rogniaux

14:25 – 573. 3D architecture of arabidopsis plant cell wall.
M. Auer

15:00 Break

15:10 – 574. Molecular mowers vs. molecular motor-mowers: The trimming of pectin by non-processive and processive methyl-esterases.
G.B. Jameson*, L.M. Kent, T.S. Loo, G.E. Norris, L.D. Melton, D. Mercadante, B. Williams

15:45 – 575. Regulation and roles of pectin methylesterases (PMEs) in plants.
L. HOQUE, F. SENECHAL, F. FOURNET, S. BOUTON, H. DEMAILLY, L. GUTIERREZ, V. LEFEBVRE, **J. PELLOUX**

16:20 Session close

Hilton Waikiki Beach
Territorial I & II

Advanced Products from Lignin and Micro- or Nano-fibrillated Cellulose (#70)

Organized by: T. Hu, A. Ragauskas, H. Hatakeyama
Presiding: H. Hatakeyama

13:00 – 576. Determining what key attributes are needed for strong lignin based carbon fibers.
A.P. Dodd, **S.K. Straus***

13:25 – 577. Control of physical properties of advanced polyurethanes derived from industrial lignins.
H. Hatakeyama*

13:50 – 578. Useful plastics with very high lignin contents should be imminent.
Y. Wang, Y. Chen, **S. Sarkane***

14:15 – 579. Unraveled enhancement of properties in polyolefin/lignin, polyolefin/cellulose nanocrystal, and polyolefin/waste cardboard biocomposites made possible by solid-state shear pulverization.
K. Iyer, G. Schueneman, **J. Torkelson***

14:40 Break

14:50 – 580. Lignin nanoparticles from tequila agave bagasse as an active component in sunscreen.
J. Gutiérrez-Hernández, N. Murillo, A. Escalante, E. Delgado, **G. Toriz***, F. Gonzalez

15:15 – 581. Green Technology for valorization of lignin: Application for production of biofuels and higher valuable small molecules.
S. Afewerkia, A. Córdova, C. Carlos-Palo Nieto

15:40 – 582. Synthesis and thermal properties of epoxy resins cured with acetylated lignin.
S. Hirose*

16:05 – 583. Agricultural biomass based catalysts for organic reactions.
X. Peng*, W. Chen, C. Wu, L. Zhong, Z. Xiang, R. Sun*

Hilton Waikiki Beach
Altitude

Chemical Ecology Applied to Sustainable Agriculture (#105)

Organized by: C. Osorio, J. Bento, T. Ando, X. Chen
Presiding: C. Osorio, J. Simões-Bento

13:00 Introductory Remarks

13:05 – 584. Sustainable management for the oriental fruit moth in pear and peach orchards in Jiangsu Province of China.
X. Chen*, M. Piao, J. Xu, G. Zhan, H. Fu

13:55 – 585. Identification and synthesis of chiral methyl-branched sex pheromones secreted by female moths.
T. Ando

14:05 – 586. Role of host-karomones and pheromones in the interaction between guava, *Psidium guajava* L. and the guava weevil, *Conotrachelus psidii* Marshall. A. Romero Frias, Y. Murata, J. Simões-Bento, **C. Osorio***

14:35 – 587. Chemical ecology of fluorescent compounds in flower pollen.
S. Mori*, M. Kawakami, M. Oishi, t. Fukui, t. Goto, J. Tsukioka, M. Osakabe, N. Sugioka, M. Sakuma, N. Hirai

Hilton Waikiki Beach
Kauai

Fate and Risks of Nanoparticles in Aquatic and Terrestrial Environments (#220)

Organized by: J. Kirby, J. Ranville, Y. Ma, B. Lee

13:00 – 588. Necessary step forward: Incorporating chemistry and spatial and temporal resolution into environmental fate models for nanomaterials.
G. Lowry*, A. Dale, E. Casman

13:40 – 589. Development of nanoinformatics tool for environmental risk assessment of nanomaterials.
Y. Tian, M. Wiesner

14:00 – 590. Influence of natural organic matter and carbon nanotube on inorganic and organic pollutant and nanoparticle toxicity: An interface point of view.
C.L. Schneider, **R. Cook***

14:20 – 591. Assessing the fate of metal-based nanoparticles in environmental matrices by single particle ICP-MS (SP-ICP-MS).
C. Stephan*, K. Wilkinson

14:40 – 592. Methods for detection and measurement of nanomaterials in and on foods.
R.B. Reed*, J. Schoepf, J. Faust, P. Westerhoff

15:00 Break

15:10 – 593. Framework for forward modeling of engineered nanomaterials in terrestrial systems.
G. Cornelis*, J. Perez-Holmgren

15:40 – 594. Measuring the mass and density of nanoparticles using Centrifugal FFF, single particle ICP-MS and TEM.
S. Tadjiki*, M. Mantano, A. Barber, J. Ranville, R. Beckett

16:00 – 595. Tracking single-wall carbon nanotubes with ICP-MS: Release from nanocomposites and biological uptake.
J. Ranville*, J. Wang, R. Lancone, H. Fairbrother

16:20 – 596. Fate of silver nanoparticles in a boreal lake ecosystem.
H. Hintelmann*, L. Furtado, C. Metcalfe

16:40 – 597. Analysis of bimetallic and polymer nanocomposites by single particle ICP-MS and field-flow fractionation.
A.G. Barber, J. Wang, M.D. Montano, S. Tadjiki, **J. Ranville**

Hilton Waikiki Beach
Prince Edward

Proteomics and Metabolomics in Agricultural, Environmental, and Public Health Sciences (#264)

Organized by: J. Johnston, Q. Li, J. Emon, J. Chen, S. Lee, C. Zhang
Presiding: S. Lee, Q.X. Li, J. Van Emon

13:00 Opening Remarks - PM Session

13:05 – 598. Blood volatile profiling for metabolomics studies.
A. de la Mata*, H. Kim, J. Harynuk

13:25 – 599. Metabolomic analysis of *Rhodococcus opacus* PD630 for its capability of paper and pulp wastewater treatment and lipid accumulation.
P. Fu*

13:45 – 600. Antibiotic-resistant metabolome and metabolites-enabled killing of antibiotic-resistant bacteria by kanamycin.
X. Peng

14:05 – 601. Analysis of potential metabolic products of asparagus bean (*Vigna unguiculata* subsp. *sesquipedalis*) under saline conditions.
L. Pan

14:45 – 602. Genome-wide investigation of diterpene biosynthesis in *Salvia miltiorrhiza* reveals rapid functional divergence of diterpene synthases.
G. Cui, L. Duan, B. Jin, R. Peters, **X. Qi***

14:45 Break

15:00 – 603. Comprehensive measurement of vitamin D metabolic markers in human serum.
D.A. Volmer*, M. Müller, C. Stokes, F. Lamert

15:20 – 604. Dissection of metabolic network in soybean seeds: From -omics data to synthetic biology.
G. Wang*

15:40 – 605. Toxicological effects of BaP, DDT and their mixture on the green mussel, *Perna viridis*, revealed by an integrated proteomic and metabolomic approach.
Q. Song, **H. Zhou***

16:00 – 606. Geochemical influences on the dental wastewater microbiome.
K.J. Rockne, A. Rani

16:20 – 607. In situ extraction of bioactive shikonins in Paterson's curse (*Echium plantagineum*) root system using polydimethylsiloxane microtubing.
X. Zhu, J. Mwendwa, J.D. Weidenhamer, D. Skoneczny, G.M. Gurr, L.A. Weston*

16:40 – 608. Quantitative proteomics analysis of high and low antioxidant expressing lines of peanut, *Arachis hypogaea*.
S. Muralidharan, Y.Y. Poon, G. Wright, N.A. Lee*

Hilton Waikiki Beach
Prince David

Analytical Development Relevant to Environmental Exposure and Effects (#288)

Organized by: C. Le, X. Li, G. Jiang, S. Richardson
Presiding: C. Le, L. Zhu

13:00 – 609. Super high through put and ultra sensitive analytical methods wanted for large-scale children's epidemiological studies.
S.F. Nakayama*

* Principle Author

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<http://pacifichem.org/onlineprogram>

- 13:20 – 610.** Volumetric absorptive micro-sampling of blood for the measurement of selected persistent organic pollutants in humans. **J. Focant***, B. L'Homme
- 13:40 – 611.** Mechanisms of ammonium assimilation by *Chlorella vulgaris* F1068: Isotope fractionation and proteomic approaches. **F. Ge***, N. Liu*, F. Li, Q. Zhou, N. Tao, M. Wong
- 14:00 – 612.** Direct measurement of pharmaceuticals and naphtenic acids through online membrane extraction coupled to mass spectrometry. **K.D. Duncan***, D. Letourneau, G. Vandegrift, E.T. Krogh, C.G. Gill
- 14:20 – 613.** Methoxylated and hydroxylated polybrominated diphenyl ethers in a marine food web from Bohai Bay, China. Y. Liu, J. Liu*, M. Yu, G. Jiang
- 14:40 – 614.** Development of sensitive analytical methods for studies on environmental exposure and effects. R. Freitas, Á. Almeida, V. Calisto, V.I. Esteves, R.J. Schneider*
- 15:00** break
- 15:20 – 615.** Addressing the challenge of bioactive contaminant identification in aquatic systems with LC/MS/QTOF. **E.P. Kolodziej***, B. Du, J.E. Baker
- 15:40 – 616.** Variation of airborne quartz in the air of Beijing during the Asia-Pacific Economic Cooperation meeting. **Q. Zhang**, G. Li, Y. Li, G. Jiang
- 16:00 – 617.** Chemiluminescence method for monitoring chemical oxygen demand and ammonium ion in water. **H.T. Do***, N. Takenaka
- 16:20 – 618.** Fate and toxicity of benzophenone-type UV filters in chlorination disinfection. **Y. Du**
- 16:40 – 619.** Metallomics study on mercury selenum interaction in rice grown in Hg contaminated field. **Y. Li***, J. Zhao, Y. Gao

Hilton Waikiki Beach
Prince Johah

Advances in Functional Foods and Flavor Chemistry Research (#329)

- Organized by: M. Qian, Z. Chen, M. Herderich, C. Wang, H. Tamura, K. Wilkinson, A. Mitchell, Q. Li
Presiding: Z. Chen, C. Wang
- 13:00** Opening remark: Introduction
- 13:05 – 620.** Conformation of cinnamic acid and its derivatives exert different strength on inhibiting tuberculosis and cancer invasion. **C. Weng***
- 13:25 – 621.** Hypocholesterolemia efficacy of quercetin rich onion juice in healthy mild hypercholesterolemic adults: A pilot study. H. Chiu, Y. Shen, K. Venkatakrishnan, C. Wang*
- 13:45 – 622.** Unexpected electrophiles in the bioactivity of curcumin. **C. Schneider***, R. Edwards, P. Luis
- 14:05 – 623.** Functional foods from ethnomyco research in Papua New Guinea. **R. Barrow***, E.M. Castillo Martinez, L. Liao, O. Kevo, A. Barish, S. Wossa
- 14:25** Break
- 14:40 – 624.** Effects of the infusion of green tea, oolong tea, and black tea on gut microbiota in a mouse model with high-fat-induced obesity. **Z. Liu, W. Zhang**, Z. Chen, L. Ni*
- 15:00 – 625.** Generation of anti-inflammatory pyroglutamyl-leucine and related peptides in rat by ingestion of enzymatic soy protein hydrolysate. **K. Sato***, A. Miki
- 15:20 – 626.** Immunomodulation of mono-saccharide conjugated ovalbumin with a tolerogenic phenotype to prevent allergic response in mice. **Y. Mine***
- 15:40 – 627.** Cholesterol-lowering activity of dietary sesamin is mediated by down-regulation on the genes involved in cholesterol absorption. **Z. Chen***, Y. Liang
- 16:00 – 628.** Health benefits of walnut consumption: Combining physiological studies with genomic and metabolomic approaches. **N.F. Shay**, t. luo, O. Miranda-Garcia, A. Hansen

- 16:20 – 629.** Iron-fortified rice and *malungay* leaves powder may impact the expression of genes associated with iron deficiency anemia and levels of blood iron concentration in pregnant Filipinas. **V.A. Timoteo***, L.M. Dalmacio, M.V. Capanzana
- 16:40 – 630.** Growth-promoting effects on intestinal probiotics in vitro by cellobiooligosaccharides from radix puerariae. **Y. Zhang***, S. Liu*, M. Zhang*, Y. Deng*, R. Zhang*, Y. Ma, Z. Wei
- 17:00** Closing remark
- Hilton Waikiki Beach
Molokai
- Radioactive Contaminants and Waste Management in the Environment (#390)**
- Organized by: W. Um, M. Baik, O. Toshihiko, A. Francis, D. Kaplan
Presiding: M. Baik, D.I. Kaplan
- 13:00 – 631.** NMR and X-ray studies of uranium-containing solid-phase precipitates. **K.T. Mueller**, W. Um, G. Wang, E. Reinosa-Maset, P. O'Day, J. Chorover, N. Washton
- 13:20 – 632.** Micro- to macroscale observation of radio cesium released from the Fukushima Daiichi Nuclear Power Plant. **K. Tanaka***, Q. Fan, A. Sakaguchi, Y. Takahashi
- 13:40 – 633.** XAS studies of radiation damage in glass - ceramic wasteforms for actinide disposition. **N. Hyatt***
- 14:00 – 634.** Behavior of technetium in nitric acid during denitrification and doping into transition metal oxides. **W. Lukens**
- 14:20 – 635.** Characterization of Fe, S, and Tc speciation within cementitious waste forms during aging underoxic and anoxic conditions. **B.A. Powell***, S. Estes, D.I. Kaplan, Y. Arai
- 14:40 – 636.** X-ray absorption spectroscopic investigation of the molybdenum speciation in the uranium mine tailings management facility at McClean Lake, Saskatchewan. P. Blanchard, J. Hayes, A.P. Grosvenor*, J. Rowson, K. Hughes, C. Brown
- 15:00 – 637.** Atomistic modeling and simulations of the Tc incorporation process into iron-oxides. **E. Kim***, P.F. Weck, W. Um, K. Czerwinski
- 15:20 – 638.** Scanning transmission electron microscopy detection of Lu incorporated in a transformation product of 2-line ferrihydrite. **T. Yokosawa***, E. Prestat, N. Finck, M. Bouby-Laliron, K. Dardenne, R. Polly, S. Haigh, M.A. Denecke, H. Geckeis
- 15:40 – 639.** Experimental determination of solubility of neodymium hydroxide in high ionic strength solutions at 298.15 K under well-constrained conditions: Comparison with model predictions. **Y. Xiong***, L. Kirkes, C. Marrs
- 16:00 – 640.** Facilitated dissolution of metal oxides by the effect of hydrazine and copper ions. **S. Kim**, W. Choi, J. Moon
- 16:20 – 641.** Transport behaviour of strontium under the effect of seawater intrusion on NPP sites. **S. Chang***, W. Um
- 16:40 – 642.** Fabrication of borate glass-ceramics to sequester lanthanide oxide wastes generated from pyro-processing technology. **M. Kim***, J. Heo
- Friday Evening**
- Hawaii Convention Center
Halls I, II, III
- Chemicals of Emerging Environmental Concern: A Global Perspective (#19)**
- Organized by: G. Cobb, J. Giesy, M. Murphy
- Poster Session**
19:00 – 21:00
- 644.** Interactions of aerosols and cloud water chemistry in the free troposphere. **H. Ogata***, H. Okochi, K. Matsunaga, S. Ogawa, Y. Minami, H. Kobayashi, K. Miura
- 645.** Effect of urban heat island on frequency and chemistry of summer heavy rainfall in downtown Tokyo, Japan. **R. Uchiyama***, H. Okochi, H. Ogata, T. Nakano
- 646.** Observation of acidic trace gases, gaseous mercury, and water-soluble inorganic aerosol species at the top and the foot of Mt. Fuji. **S. Ogawa***, H. Okochi, H. Ogata, T. Nagoya, H. Kobayashi, K. Miura, Y. Minami, S. Kato, S. Yonemochi, N. Umezawa
- 647.** Formation of volatile carbonyls from electronic (e-) cigarette carriers. **P. Wang**, W. Chen, T. Matsuo, K. Ito, J. Fowles, k. Kumagai
- 648.** Method of reducing the elution of arsenic from gypsum by use of iron-based agent. **D. Yang**, A. Sasaki, M. Endo
- 649.** Flocculation of emulsified oil using a novel amphiphilic and cationic chitosan-based flocculant. **T. Lyu***, H. Zhao, D. Zhang
- 650.** Effects of environmental factors on the degradation on neonicotinoids. **M.M. McManus**, A.M. Cano, S. Deleon, J.D. Maul, J.E. Canas-Carrell*
- 651.** Geospatial analysis of lead in American woodcock. **A. French***, D. Sullins, W.C. Conway, D. Klein
- 652.** Arsenic uptake by Muskmelon (*Cucumis melo*) fruits from contaminated water. **B.E. Hettick***, D. Klein
- 653.** ZnO nanoparticles exposure induces developmental toxicity in embryo-larval zebrafish. **J. Cho***
- 654.** Expanded polystyrene debris as a source of toxic substance, hexabromocyclododecanes, in the marine environment. **S. Hong***, M. Jang, M. Rani, W. Shim, G. Han, Y. Song
- Hawaii Convention Center
Halls I, II, III
- Chemical Ecology Applied to Sustainable Agriculture (#105)**
- Organized by: C. Osorio, J. Bento, T. Ando, X. Chen
- Poster Session**
19:00 – 21:00
- 655.** Effect of hydrogen on plant growth subjected to salinity stress. **T. YAMAOKA***, Y. Kurita, S. Okouchi, T. Antonio, R. Okajima
- 656.** Overview of research and application of insect pheromones in China. **X. Chen**, C. Sheng*
- 657.** Radiation application for environmental pollution prevention. **T. Kim***, J. Kim, S. Lim
- 658.** Browning mechanism on the roots of rice plant attacked by rice root aphid, *Rhopalosiphum rufiabdominalis*, and effects of salicylic acid. **A. Mori**, S. Tebayashi, S. Ueda, A. Okawa, R. Sasaki, M. Uwate, H. Maseda, K. Saito, A. Ishihara
- 659.** Insect growth inhibitor from *Itea virginica*. **K. Seo**, S. Tebayashi, M. Hiroshima, S. Oonishi, M. Sato, T. Hukuda
- 660.** Regulation of flavonoid production in the leaves of bell pepper by light condition. **S. Tebayashi***, Y. Takeo, S. Oonishi, K. Yoshida
- Hawaii Convention Center
Halls I, II, III
- Fate and Risks of Nanoparticles in Aquatic and Terrestrial Environments (#220)**
- Organized by: J. Kirby, J. Ranville, Y. Ma, B. Lee
- Poster Session**
19:00 – 21:00
- 661.** Concentration-dependent influence of engineered magnetic nanoparticles on the disinfection of fecal coliforms in wastewater effluent. **V. Hwang***, E. Montalvo
- 662.** Transport and removal of nanoparticles with water in porous media. **X. Li***, G. Hui
- 663.** Differential effect of ZnO NPs and Zn ions on corn seedlings at different temperatures: enzyme activity, protein production, and Zn biotransformation. **G. de la Rosa**, L. Lopez, G. Cruz-Jimenez, L. Castellanos-Torres, J. Gonzalez-Chavez, K. Sanchez-Sánchez, J. Gardea-Torresdey
- 664.** Oxidative dissolution of silver nanoparticles in presence of free chlorine. **S. Garg***, H. Rong, C.J. Miller, T.D. Waite
- 665.** Fate and transport of TiO₂ and ZnO in similar environmental conditions. **S. Al-Abed***
- 666.** Observation of fine particles at the summit of Mt.Fuji, 2013-2015. **S. Oishi***, S. Yonemochi, M. Murata, H. Okochi, T. Nagoya
- 667.** Direct interaction of Fe(II) complexes with inorganic/organic hybrid sheaths of *Leptothrix*, Fe-oxidizing bacterium. **T. Kunoh***, K. Tamura, H. Kunoh, J. Takada
- 668.** Characterization of fine and ultrafine particles in urban, forest, and mountainous site in Japan. **K. Matsunaga***, H. Okochi, H. Ogata, T. Nagoya, K. Adachi, y. zaizen, Y. Igarashi, A. Miyazaki
- Hawaii Convention Center
Halls I, II, III
- Proteomics and Metabolomics in Agricultural, Environmental, and Public Health Sciences (#264)**
- Organized by: J. Johnston, Q. Li, J. Emon, J. Chen, S. Lee, C. Zhang
- Poster Session**
19:00 – 21:00
- 669.** Proteomic analysis of *Pinctada martensi* up on exposure to benzo[a]pyrene. **H. Chen***, Q. Song, X. Diau
- 670.** New, easy-to-use, automated, and fast method for biomarker discovery. **A. de la Mata**, L. Adutwum, A. Mani-Varnofaderani, J. Harynuk
- 671.** Proteomics profiling of *Bacillus licheniformis* reveals metabolic mechanism in synthesis of extracellular polymeric flocs. **N. He***, W. Yu, L. Shen, Y. Wang
- 672.** CuO/TiO₂ photocatalysts for highly efficient and rapidly debromination of decabromodiphenyl ether. **M. Lei**, Q. Zhou, H. Tang
- 673.** Qualitative and quantitative proteomics of legume-symbiont *Mesorhizobium loti*. **Y. Tatsukami**, M. Nambu, H. Morisaka, K. Kuroda, M. Ueda
- 674.** Differential regulation to OmpC and OmpF between nalidixic acid- and chlorotetracycline-resistant *Escherichia coli*. **S. Wang**, X. Lin, X. Peng
- 675.** Ni doped graphitic-like carbon nitride nanoplate based electrochemical sensor for the determination of octylphenol environmental water samples. **J. Zou***, w. Gong, S. Zhang, X. Zhou
- 676.** Rapid analysis of tetracyclines and sulfonamides in chicken meat by on-line solid phase extraction-high performance liquid chromatography coupled with accelerated solvent extraction. **Q. Zhou**, M. Lei, L.h. Zhu, H.q. Tang

* Principle Author

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677. Rapid biodegradation of organophosphorus pesticides by *Stenotrophomonas* sp. G1. S. Deng, **R. Hua**, X. Tang, X. Wu, H. Cao, X. Li, J. Tang

Hawaii Convention Center
Halls I, II, III

Analytical Development Relevant to Environmental Exposure and Effects (#288)

Organized by: C. Le, X. Li, G. Jiang,
S. Richardson

Presiding: X. Li, S. Richardson

Poster Session
19:00 – 21:00

678. Role of EPS from *Chlorella vulgaris* in the removal of ammonium and orthophosphate under the stress of cadmium. **B. Chen***, F. Li*, N. Liu, F. Ge, H. Xiao, Y. Yang

679. Estimation of heavy metals captured by Konara (*Quercus serrata Murray*) canopy in a small forest ecosystem in the Greater Tokyo area using a leaf washing method. M. Yoshida, H. Okochi, **A. Miyazaki***

680. Capillary electrophoresis-mass spectrometry characterization of water samples derived from Athabasca lean oil sands and mixed surficial materials. M.S. MacLennan, J.V. Headley, K. Peru, C. Swyngedouw, I. Fleming, **D.D. Chen***

681. Evaluation of RAR binding activity materials in Azolla to inhabit the reservoir with yeast two hybrid assay. **A. Sawabe***, S. Mukai, R. Takeda, A. Iida, D. Nakajima, F. Shiraishi

682. Atmospheric behavior and health risk assessment of polycyclic aromatic hydrocarbons in urban, forest, and mountain-site in Japan. **K. ONO***, H. Okochi, H. Ogata, Y. Minami, H. Kobayashi, K. Miura, S. Kato, K. Matsuda

683. Pyrethroid pesticide pollution of hard clams in an estuary adjacent to industrial areas. **M. Goto***, T. KANEKO, R. TAKANASHI, Y. MANAKA, T. FURUHATA

684. Composition and particle size distribution of particulate fatty acids derived from thermal cooking. **N. Shinomiya***, A. Miyazaki, N. Tanaka

685. Composition and particle size distribution of PAHs generated by thermal cooking: Effect of cooking equipment and heat sources. **N. Tanaka***, E. Saito, M. Tsuzaki, A. Miyazaki

686. Occurrence, estrogenic activity, and toxicity of emerging bisphenol analogs. M. Song*, T. Ruan, **G. Jiang**

687. Age, smoking, and radiation effects on the production of reactive oxygen species in blood cells of atomic-bomb survivors and their association with immune-related biomarkers. **T. Hayashi***, K. Furukawa, W. Ohishi, I. Hayashi, K. Yoshida, S. Kyoizumi, Y. Kusunoki, K. Nakachi

688. Development and application of a simultaneous measurement method for gaseous ammonia and particulate ammonium in ambient air. **H.H. Duong***, N. Takenaka*

689. Production control of edible mushrooms by the specific irradiation of blue light LED. **Y. Miyazaki***, S. Kaneko, Y. Sakamoto, M. Nakamura

690. Role of urban small forest on air pollution reduction and VOCs emission in the Greater Tokyo, Japan. **C. Aso***, H. Okochi, H. Ogata, A. Miyazaki

691. Observation of dry deposition of acidic substances onto the forest canopy in a small conifer/deciduous mixed forest in greater Tokyo using foliar rinsing and surrogate surface method. **Y. Sugiyama***, H. Okochi, A. Miyazaki, H. Ogata

692. Fractionation and determination of glycidol, 3-MCPD, glycidyl fatty acid esters and 3-MCPD fatty acid esters in infant formula. **T. Fukazawa***, H. Kido, S. Wada, T. Maruyama

693. Interannual change, seasonal variations, and the size distribution of anionic surfactants in particulate phase in downtown Tokyo, Japan. **R. Hirokawa***, H. Okochi, H. Ogata, M. Soda

694. New sensitive method for the determination of trace hydroxylamine in environmental water using hypochlorite, followed by gas chromatography. **Y. SEIKE***, S. SUGAHARA, Y. SENGA, M. Egawa, H. KAMIYA, M. OKUMURA

695. Geographic distribution and interannual change of trace metals in stream water in the east Tanzawa mountains and the effect of atmospheric deposition.

K. Shinmen, H. Okochi, R. Aoki, H. Ogata

696. Simultaneous determination of urinary cotinine and an oxidative stress marker (8-OHDG) by on-line column switching liquid chromatography tandem mass spectrometry. **Y. Onoda**, M. Yoshikane, F. Mizutani, N. Sato

697. Study on determination of inorganic nitrogen in the presence of residual chlorine. **M. Egawa**, S. SUGAHARA, Y. SEIKE*

698. In-cloud and below-cloud scavenging of polycyclic aromatic hydrocarbons and their dry deposition onto forest canopy. **H. Okochi**, H. Ogata, M. Fujita, G. Rossini, Y. Minami

Hawaii Convention Center
Halls I, II, III

Advances in Functional Foods and Flavor Chemistry Research (#329)

Organized by: M. Qian, Z. Chen, M. Herderich, C. Wang, H. Tamura, K. Wilkinson, A. Mitchell, Q. Li
Presiding: Z. Chen, A.E. Mitchell

Poster Session
19:00 – 21:00

Opening remark

699. Pyrolysis GC-MS of fractionated tobacco extracts for the in-depth study of aroma compounds. **K. Mitsui***, F. David, P. Sandra, H. Tamura

700. Metabolomics approach to thermal changes in the flavor profile of tomato juice as a cooking model. **Y. Iwasaki***, Y. Atagiri, T. Sato, H. Otomo, A. Obata, Y. Iijima

701. Scale down quick, easy, cheap, effective, rugged and safe method for the determination of 3-alkyl-2-methoxy-pyrrazines in wines by gas chromatography-mass spectrometry. **A.R. Fontana***, R. Bottini

702. Screening discrimination of snack confectionery with fragmentless ionization mass spectrometry. **T. TSUGOSHI***, Y. Kato, Y. Mishima

703. Development of a high-performance liquid chromatography method based on a core-shell column approach for the rapid quantification of polyphenols in grape pomaces. **A.R. Fontana***, A. Antonioli, R. Bottini

704. Strategy for evaluating food functionality: Application of MALDI-MS to high-throughput metabolic profiling of green tea extracts with antioxidant activity.

Y. Fujimura*, E. Hayakawa, D. Miura, H. Warishi, H. Tachibana

705. Applying laser Doppler vibrometer to detection of watermelon texture. **Z. Gao**, D. Cui

706. Analysis of organic acids in sake using gas chromatography. **C. Kohsaka***, K. Hirooka, Y. Yamamoto, K. Ichihara

707. Isotope dilution LC-MS method for the quantification of curcumin and its metabolites in human plasma. **C. Schneider***, P. Luis

708. 3-Methylbutanol glycosides in raw *Coffea arabica* beans are potent determinants of coffee beverage quality.

K. Iwasa*, D. Setoyama, H. Shimizu, H. Seta, Y. Fujimura, D. Miura, H. Warishi, C. Nagai, K. Nakahara

709. Selective reduction of aged odor in Japanese sake by supported noble metal nanoparticles. **Y. YAMAMOTO**, T. HASEGAWA, H. Murayama, T. ISHIDA, A. ISOGAI, T. FUJII, **M. Tokunaga**

720. Basic study on contaminated cooling seawater in Fukushima NPP: Behavior of fission products leached from neutron-irradiated uranium oxide solid solutions.

T. Sasaki*, Y. Takeno, T. Kobayashi, A. Kirishima, N. Sato

721. Taste properties of theanine. **M. Narukawa***, Y. Toda, T. Nakagita, K. Morita, Y. Hayashi, T. Misaka

722. Comparison of tea catechin polymers generated by enzymatic and chemical oxidation, microbial fermentation, roasting, and treatment with herbal essential oils. Q. Hao, T. Shii, S. Teramoto, A. Inada, **Y. Matsuo**, T. Tanaka*

723. Neuroprotective compounds from corn silks alleviate amyloid cytotoxicity in SH-SY5Y cells. **Z. Liang**, Q.X. Li*

724. Antioxidant activity and cytotoxicity of black rice extract. **K. Seo***, J. Lee, y. Lee, T.K. Park, B. Lim

725. Searching for functional foods for prevention of Alzheimer's disease.

S. Matsumura, Y. Yoshioka, Y. Ueno, T. Furuta, **K. Murata**, H. Matsuda*

726. Effects of a newly found active ingredient, Fragilein, in Jenzhang vinegar, on a model mouse of dietary obesity.

Y. TSUJINO*, M. TAKAGI, Y. YOSHIDA, N. Gotoh, A. Satoh

727. Protective effects of dietary 1,5-Anhydro-D-glucitol in diabetes and metabolic syndrome. **A. Katō***, K. Tomomura, I. Adachi, F. Ishikawa, K. Takeshita, J. Hollingshead, R. Nash, Z. Liu, S. Jenkins, G.W. Fleet

728. Prevention of the photobleaching of chlorophyll using antioxidants and surfactant Triton X-100. **M. Yasuda***, M. Tabata

729. Potential use of Katsubushi processing residues as nutritional supplements or antioxidant sources. **D. Meng***, G. Kasane, H. Endo, H. Ren*

Closing remark

Hawaii Convention Center
Halls I, II, III

Fukushima and Radiological Contaminated Environments World-wide: The Important Role of Environmental Chemistry and Radiochemistry in Remediation and Restoration (#374)

Organized by: T. Sasaki, H. Nitsche, C. Liu, Z. Yoshida, S. Kalmykov, L. Rao

Poster Session
19:00 – 21:00

730. Activity concentrations of radio cesium in Tamagawa River Watershed, western district of Tokyo after the Fukushima Daiichi Nuclear Power Plant accident.

K. Ochi, Y. Kurihara, R. Aobayashi, K. Hagiwara, N. Nagawa, T. Nakamura, Y. Koike*

731. Seasonal change of radio cesium and potassium concentrations in Someiyoshino cherry and Japanese chestnut trees observed after Fukushima nuclear accident.

K. Tagami*, S. Uchida

732. Radioactive contamination of the Tokyo metropolitan area by the Fukushima Daiichi Nuclear Power Station accident.

H. Yamazaki, M. Ishida, W. Ishii, K. Takashimizu, K. Honda

733. Ab initio description of the changes induced by radioisotopic transmutations in Fukushima soil minerals.

M. Sassi, K. Rosso, M. Okumura, S. Kerisit, M. Machida

734. Basic study on contaminated cooling seawater in Fukushima NPP: Behavior of fission products leached from neutron-irradiated uranium oxide solid solutions.

T. Sasaki*, Y. Takeno, T. Kobayashi, A. Kirishima, N. Sato

735. Dynamics of radioactive cesium in fish by the Fukushima Daiichi Nuclear Power Station accident and their environmental consequence in aquatic ecosystem.

M. Ishida*, T. Ikeuchi, K. Takashimizu, H. Yamazaki

736. Thermodynamic study of the complexation of humic acid by calorimetric titration.

S. Kimuro, A. Kirishima, **A. Kirishima***, D. Akiyama, N. Sato

737. Electro-occlusion of cesium into a porous aluminum plate. **T. Ihara***, H. Yamanishi, N. Tanaka, H. Noma, T. Ito

738. Pu contamination in surface soils after the Fukushima Daiichi Nuclear Power Plant accident. **M. Yamada***, T. Yamaguchi, H. Tazoe, Y. Hosokawa

739. Decontamination system for radionucllear contaminated water caused by Fukushima Daiichi nuclear disaster.

K. Yokota, H. Ogawa, M. Iwasa, K. Fukunishi, M. Ito, T. Otsu, H. Yoshida, R. Nakamura

740. Relation between adsorption/desorption characteristics of cesium ions onto the rocks and components. **T. Miura**, N. Takizawa, A. Sasaki, M. Endo

741. Study on Cs(II) adsorption and desorption on suspended matters in Fukushima river water. **M. Onodera**, A. Kirishima, D. Akiyama, N. Sato, S. Nagao

742. Development of radioactive cesium absorbent using chitosan-modified rayon fiber. **S. Omote**, T. Furukie, H. Tamura*

743. Effect of contact time, pH, ionic strength, coexisting ions and humic substances on the sorption of uranium(VI) on kaolinite. **X. Wang***, S. Li*, L. Du, Z. Tan, X. Wang

744. Dry, non-heated decontamination of radioactive cesium polluted soils using paramagnetic Fe₃O₄. **Y. Mitoma***, C. Simion, S.R. Mallampati, T. Okuda, K. Nakata

745. Sorption of uranium(VI) on GMZ bentonite: Effect of pH, ionic strength, foreign ions, and humic substances. S. Li*, **X. Wang***, Z. Huang*, L. Du, Z. Tan

736. Sorption behaviors of ¹²⁵I⁻ on Beishan granite and Gaomiaozi bentonite. C. LIU, X. Yang*, J. He, W. Tian, B. Ma

737. Leaching of actinide elements from simulated fuel debris to seawater and pure water. **M. Hirano***, A. Kirishima, N. Sato, T. Sasaki

738. Adsorption properties of cesium to micaceous clay minerals: Molecular modeling using density functional theory calculations. **M. Okumura***, H. Nakamura, M. Machida, M. Sassi, K. Rosso

739. Environmental dynamics of dissolved radionuclides and ions in riverine water after the FDNPP accident. **R. Tomita**, T. Matsunaka, M. Honda, Y. Satou, M. Matsumura, T. Takahashi, A. Sakaguchi, H. Matsuzaki, K. Sasa, K. Sueki

740. Concentrate of radioactive iodine in inland water to water plant. **T. Masaomi**, H. Yamamoto, H. Momose

741. Time variation of iodine-129 and radioactive cesium in river water at Ohori River. **K. Sueki**, N. Shibayama, R. Tomita, Y. Satou, K. Sasa, T. Takahashi, T. Matsunaka, M. Matsumura, H. Matsuzaki, M. Murakami, R. Yamashita, H. Takada, Y. Koibuchi, H. O. G. Moura, T. Oki

742. Distribution of the atmospherically deposited radioactive cesium in small forest in Fukushima prefecture and development of ecofriendly technology for its decontamination. **S. Kinno**, H. Okochi, H. Kuroshima, H. Ogata, M. Hosoda, S. Tokonami, A. Soraishi, M. Kataoka, A. Kishimoto

743. Inhibitory effects for the desorption of absorbed Cs⁺ from the natural zeolite. **K. Togashi**, N. Takizawa, A. Sasaki, M. Endo

* Principle Author

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744. Simulating the interaction between humic acid and uranyl. **D. Wang***, Z. Chai, H. Wang, T. Lan

Hawaii Convention Center
Halls I, II, III

Radioactive Contaminants and Waste Management in the Environment (#390)

Organized by: W. Um, M. Baik,
O. Toshihiko, A. Francis, D. Kaplan
Presiding: W. Um

Poster Session 19:00 – 21:00

745. Detection efficiency curve using three commercially available chemical reagents for gamma-ray spectrometry. **R. Suzuki**, Y. Kurihara, Y. Iwahana, T. Nakamura, Y. Koike*

746. Uranyl peroxide cage cluster interactions at mineral interfaces. **C. Dorais***, A.E. Hixon

747. Immobilization of volatile ^{129}I by vitrification. **C. Lee***, J. Heo

748. Thermodynamic properties of Tc retention in magnetite. **M. Lee**, W. Um, V. Glezakou*

749. Study of colloid facilitated transport of contaminates in a microscale saturated porous media analog. **Y. Guo***, J. Huang, X. Yin, K. Neeves, N. Wu

750. Impacts of physical and chemical heterogeneities on radionuclide-carrying colloids transport in saturated porous media. **G. Wang**, W. Um, J. Chun

751. Fracture flow of radionuclides in unsaturated conditions at Wolsong LILW Disposal Facility, South Korea. **W. Kim***, J. Kang, J. Kim, S. Nam, H. Jung, W. Um

752. Recovery of cesium using a thixotropic gel. **T. Watanabe***, T. Saito

753. Consideration of water radiolysis in void volumes of porous zeolite bed loaded in adsorption vessels for decontamination of radioactive water. **R. Nagaishi***, M. Inoue, T. Matsumura, I. Yamagishi, R. Hino, T. Ogawa

754. Transport behavior of ^{137}Cs , ^{90}Sr and ^{99}Tc in the proposed near surface repository in Wolsong Site, South Korea. **J. Kim***, W. Kim, S. Choi, M. Kwon, W. Um

755. Functional engineered barriers: A mineralogical approach to improved radionuclide sorption. **C.L. Corkhill***, J.W. Bridge, D.E. Crean, J.E. Vigor, R. Tappero, C.A. Murray, C. Tang, N. Hyatt

756. New Technetium-99 LSC counting methodology for environmental and radiopharmaceutical analysis. **M. Khan***, W. Um*

757. Thorium waste immobilization in hierarchical zeolite prepared from natural resources through tandem acid-base treatment. G. Nurlati, **Y.K. Krisnandi***, R. Sihombing, Z. Salimin

758. Adsorption of Th^{4+} on temperature sensitive urea-formaldehyde resin and its regeneration by extraction separation. **S. Tang***

759. Adsorption properties of Ag^+ and Ce^{4+} in nuclear power plant wastewater by urea-formaldehyde chelating resin. **S. Tang**

760. Uranium immobilization by plant roots in acidic wetlands. **D. Li***, D.I. Kaplan, J. Seaman, H. Chang, P. Jaffé, K. Scheckel, C. Segre

761. Mercury speciation in Savannah River Site high-level waste: Determination and implications for waste handling and disposal. **C.J. Bannochie***, C.L. Crawford, M.M. Reigel, P. Garcia-Strickland

762. Low temperature hydrothermal synthesis of soil into pollutants to immobilize radioactive Cs. **J. Fan**, Z. Jing, F. Jin

763. Synthesis of phosphate functionalized magnetic mesoporous carbon for sequestering of uranium. **S. Husain**, W. Um*, Y. Chang*

764. Synthesis of amine impregnated mesoporous silica for radioactive iodine gas removal. **S. Han***, J. Kang, W. Um

765. Immobilization of strontium via strontianite (SrCO_3) precipitation by aerobic microorganism enriched from rhodoliths. **S. Kang**, Y. Roh

766. Removal of strontium ions from aqueous solution by the adsorption onto Okara. **R. Ikeda**, H. Sakano, K. Omata, H. Shimofuruya*

767. Temporal variation of microbial community in low- and intermediate-level radioactive waste(LILW) disposal facility in Republic of Korea. **J. Ahn***, W. Kim, J. Park, W. Um

768. Leaching characterization methods applied to core samples from an engineered scale demonstration of a prospective cast stone process. **C.L. Crawford***, A.D. Cozzi, D.J. Swanberg

769. Removal of refractory compounds from stabilized leachate using low-cost coconut shell waste-based activated carbon modified with ozone. **T.A. Kurniawan***

770. Organic apatite synthesis and application for uranium removal. **H. Kim***, W. Um

771. Soil-soil solution partitioning coefficient of Mn-54 in Japanese agricultural fields. **S. Uchida***, K. Tagami

772. Chemical decontamination process for Challe River unidentified deposit (CRUD) removal. **S. Nam***, W. Kim, W. Um

773. Solubility of Niobium in aqueous solution under high pH conditions. **H. Iwata***, A. Kitamura

774. Effect of iron oxides on the rheology of cementitious paste. **C. Chung**, J. Chun, G. Wang, W. Um

775. Effect of curing condition on immobilization of cesium in waste incineration fly ash by geopolymmerization. **M. Takaoka***, T. Nakamura, K. Shiota, T. Fujimori, K. Oshita

Saturday Morning

Hilton Waikiki Beach
Territorial III

Pectin Chemistry and Technology (#20)

Organized by: B. Savary, M. Williams, S. Lu, S. Yoo, R. Cameron

8:00 Opening

8:05 – 776. Presence of proteoglycans containing apiose-rich pectin, xylan, and arabinogalactan in *Spirodela polyrhiza*. **L. Tan***, E. Hunt, J. Qian, G. Huang

8:35 – 777. Epitope detection chromatography: A new method to study pectin heterogeneity. **V. Cornault**, P. Knox

9:05 – 778. Technological application for pectin methylesterase activity inhibition in tropical fruits. **P. Vasu***

9:35 – 779. Structure-function analyses of tomato and strawberry pectic polysaccharides in relation to fruit textual properties during ripening. **S. Pose***, P. Knox

10:05 Break

10:15 – 780. Composition and structure of pectic material from frozen concentrated orange juice and characterization of its molecular structural changes during juice cloud destabilization. **A. Galant**, Y. Kim, G.a. Luzio, W. Widmer, **R. Cameron**

10:45 – 781. Fibergel Ic® - novel gelling fiber for texture development in foods. **E.P. Anders***

11:15 – 782. Composition and rheological properties of processed citrus fiber. **B. Lundberg***, x. pan, A. Hotchkiss

11:45 Close

Hilton Waikiki Beach
Hawaii

Human Exposure to Environmental Contaminants (#26)

Organized by: J. Martin, K. Kannan, L. Zhu, H. Moon
Presiding: K. Kannan, J. Martin

8:00 – 783. Chemical-specific exposure assessment at EPA: Case studies on dioxin, PBDEs, and DEHP. **M. Lorber***

8:40 – 784. Assessing exposure to persistent and emerging environmental contaminants in the Australian population with an emphasis on early life exposures.

J. Mueller*, A. Heffernan, Y. Chen, C. Baduel, M. Gomez Ramos, P. Thai, P. Hobson, S. Broomhall, L.L. Toms

9:00 – 785. Meconium and placenta as a non-invasive human tissue for prenatal exposure to persistent organic pollutants (POPs). **Y. Jeong**, S. Lee, s. kim, j. park, K. Choi, s. kim, H. Moon*

9:20 – 786. Maternal urinary concentrations of free and total bisphenol A (BPA) and BPA-alternatives in the APRON birth cohort. **J. Liu**, C. Field, I. Dinu, D. Dewey, J. Martin*

9:40 – 787. Occurrence of phthalate diesters (phthalates), *p*-hydroxybenzoic acid esters (parabens), bisphenol A diglycidyl ether (BADGE), and their derivatives in indoor dust from Vietnam: Implications for exposure. **T.M. Tran***, T.B. Minh, T.A. Kumasani, K. Kannan

10:00 – 788. Biomonitoring of human exposure to endocrine disrupting chemicals in the United States. **K. Kannan**

10:20 – 789. Application of thermodynamic activity to assess human exposure and health risks of phthalate esters in consumer products. **F.A. Gobas***, L. Tupper-Ring, V. Susan

10:40 – 790. Role of biofilm roughness and hydrodynamic conditions in *Legionella pneumophila* adhesion to and detachment from simulated drinking water biofilms. **Y. Shen**, H. Nguyen*

11:00 – 791. Arsenic in wine and other alimentary items. **I. Koch***, M. Mills, K. House, J. Sui, J. Zhang, M. Nearing, K. Reimer, D. Loock, K.P. Weber

11:20 – 792. Estrogenic exposure in human from the photochemical transformation of typical emerging organic contaminants in water. **Y. Gao**, G. Li*, Y. Ji*, **T. An***

Hilton Waikiki Beach
Territorial I & II

Recycling of Polymeric Materials: Challenges and Perspectives (#36)

Organized by: T. Yoshioka, K. Joo-Sik, V. Sahajwalla, B. Thallada

8:00 Opening

9:00 – 793. Production of a hydrogen-rich syngas with low tar and ammonia from steam/oxygen gasification of dried sewage sludge in a two-stage gasifier. **Y. Choi***, J. Kim

9:20 – 794. Recycling waste polymers in ironmaking: Fundamental investigations on thermal degradation, structure evolution, and carbon dissolution. **R. Khanna***, V. Sahajwalla

10:00 – 795. Recycling technology of fiber reinforced plastics using subcritical fluidics. **M. Goto***, T. Nakagawa

10:40 – 796. Decrosslinking of crosslinked polyethylenes via ultrasonically aided extrusion technologies. **A.I. Isayev***

11:00 – 797. Transforming electronic waste into value-added materials. **R. Rajagopal***

11:20 – 798. Efficient conversions of plastics into economically valuable products. **A. Kamimura***, H. Matsumoto, K. Ikeda, K. Kaiso

Hawaii Convention Center
Halls I, II, III

Advanced Products from Lignin and Micro- or Nano-fibrillated Cellulose (#70)

Organized by: T. Hu, A. Ragauskas, H. Hatakeyama
Presiding: T. Hu

Poster Session

10:00 – 12:00

799. Thermal properties of kappa-carrageenan hydrogels filled with micro fibrillated cellulose. **M. Iijima***, T. Hatakeyama, H. Hatakeyama

800. Synthesis and thermal properties of cross-linked epoxy resins with ester chains derived from glycidylated lignin. **M. Masuda***, S. Hirose

801. Novel epoxy resins with ester chains derived from lignin and cyclic compound. **M. Shimizu***, K. Zaito, D. Yamane, S. Inada, S. Hirose

802. Synthesis of lignoalkanes from lignocresols with a Ca-Rh/C-EtOH system and their application as polymer compatibilizer. **Y. Mitoma***, M. Aoyagi, N. Egashira, C. Simon, **D. Yokoyama**

803. Thermal conductive properties of nanocellulose materials. **T. Okada***, K. Uetani, H.T. Oyama

804. Fluorescent property of CMC/Tb nanocomposites in different pHs. **J. Ye**, Q. Li, J. Xiong

805. Use of ultrasonic technology in the catalysis of the TEMPO oxidation for the nanofibrillation of Kraft pulp: Reinforcement of nanocomposites materials. **C. Daneault***

806. Characterization of lignin-carbohydrate complex linkages using nuclear magnetic resonance spectroscopy. **H. Nishizuma***, A. Kamiya, M. Katahira, T. Watanabe

807. Composition of cellulosic fibers and lignin based on acidification of black liquor. **H. Nonaka***, T. Kato

808. Horseradish peroxidase modification of sulfomethylated alkali lignin to improve enzymatic saccharification of lignocelluloses. **D. Yang**, Y. Chang, H. Lou, X. Qiu*, **Y. Qian***

809. Cellulose nanofibres-polyvinyl alcohol nanocomposite films with improved mechanical strength. **C. Yadav**, **P. Mohanty***

810. Pickering emulsion stabilized using amphiphilic cellulose nanofibers prepared by the aqueous counter collision method. **K. Kamada**, S. Yokota, T. Kondo*

811. Cellulose/chitin nanowhiskers stabilized sterically by grafted polymer brushes. **J. Araki***

812. Preparation of lignin microsphere and its adsorption performance towards lead ions from aqueous solution. **Z. Li***, Y. Ge*

813. Characterization of biocompatible materials produced by nanofibrillation and surface modification of cellulose. **F. Tani***, K. Abe, T. Masuda, K. Matsumiya, Y. Nanbu, Y. Kase, D. Kamitaka, K. Fujiwara, S. Kikkawa, N. Ishii, M. Ryu, Y. Suzuki, Y. Matsumiya, H. Watanabe, Y. Matsumura, H. YANO

814. High-resolution solution-state NMR analysis of wood, cellulose, and surface-modified nanocelluloses in ionic liquid electrolytes. **A. Holding**, J. Helminen, V. Mäkelä, E.I. Filpponen, I. Kilpeläinen, **A.W. King**

Hilton Waikiki Beach
Alitude

Chemical Ecology Applied to Sustainable Agriculture (#105)

Organized by: C. Osorio, J. Bento, T. Ando, X. Chen
Presiding: T. Ando, J. Simões-Bento

8:00 Introductory Remarks

8:05 – 815. Design, synthesis, and insecticidal activity of novel oxadiazine derivatives. **D. Xu***

* Principle Author

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8:35 – 816. Autoxidation of longifolene and antitermite activity of its products.
A. Mukai*, T. Ashitani, K. Takahashi
9:05 – 817. Manipulation of (2E)-hexenal production in plants to elucidate its roles under biotic and abiotic stress conditions.
M. Kunishima, Y. Yamauchi, M. Mizutani, Y. SUGIMOTO

Hawaii Convention Center
Halls I, II, III

Elements Essential to Biosphere Health: Bioremediation and Biogeochemical Cycling (#219)

Organized by: L. Eltis, M. Fukuda, L. Wackett

Poster Session
10:00 – 12:00

818. Expression of the bacterial heavy metal transporter MerC fused with a plant SNARE in *Arabidopsis thaliana* increases mercury accumulation.
M. Kiyono*, Y. Sone, R. Nakamura, Y. Takanezawa, S. Uraguchi

819. Role of Mer in the transport of mercurials in *Escherichia coli*.
Y. Sone, R. Nakamura, Y. Takanezawa, S. Uraguchi, M. Kiyono*

820. Aerobic reduction of selenite by a filamentous fungus, *Aspergillus oryzae* for selenium recovery and recycling.
T. Sakaguchi*, H. Kimura, M. Nagaoka, T. Arima, Y. Okamura, M. Maeda

821. Identification and characterization of a novel *N*-acylhomoserine lactonase from coagulase-negative staphylococci.
R. Sato*, T. Yamaguchi, N. Someya, T. Ikeda, T. Morohoshi

822. Identification and characterization of a novel *N*-acylhomoserine lactonase from plant-associated bacteria.
T. Yamaguchi, S. Kikuchi, N. Someya, T. Ikeda, T. Morohoshi

823. Identification and characterization of a novel *N*-acylhomoserine lactonase from activated-sludge bacteria.
S. Yasumoto*, S. Ochiai, T. Morohoshi, T. Ikeda

824. Biological hydrolysis and acidification of iron-enhanced primary wastewater sludge under an anaerobic condition: Effects of pH, temperature, and the substrate concentration.
X. Li*, R. Li, H. Li, Y. Li, J. Xu

825. Transformation and products of thiol drugs with the presence of humic substance in water during enzymatic catalysis.
P. Du, H. Zhao, H. Cao

826. Enzymatic activity of cell-free extract from *Geobacillus* sp. UZO 3 catalyzes reductive cleavage of diaryl ether bonds of 2,3,7,8-TCDD.
M. Nakamura*, Y. Otsuka, Y. Miyazaki, Y. Suzuki, Y. Katayama, T. Kameyama

Hilton Waikiki Beach
Kauai

Fate and Risks of Nanoparticles in Aquatic and Terrestrial Environments (#220)

Organized by: J. Kirby, J. Ranville, Y. Ma, B. Lee

8:00 – 827. Dose and duration of manufactured nanoparticle exposure in ecosystems influences nanoparticle fate and impacts.
B.P. Colman*, L. Baker, C. Matson, R. King, C. Richardson, E. Bernhardt

8:40 – 828. Screening method for the eco-toxicological effects of engineered nanomaterials on microbial communities in terrestrial and aquatic environments.
K.P. Weber*

9:00 – 829. Effects of nanomaterials on soil microbial communities, plant-rhizobia symbiosis, and mycorrhizal colonization of plant roots in biosolid-amended soil.
J. Judy*, J. Kirby, M. McLaughlin, P. Bertsch

9:20 – 830. Determination of uptake and bioaccumulation of multi-walled carbon nanotubes in *Daphnia magna* and *Pimephales promelas* using microwave induced heating.
A.M. Cano*, M. Saed, M. Green, J.D. Maul, J.E. Canas-Carrell
9:40 – 831. Trans-generational impact of silver sulfide nanoparticles on the earthworm *Eisenia fetida*.
J. Kirby, J. Judy, D. Navarro
10:00 Break
10:15 – 832. Long-term effects of silver nanoparticles on activated sludge.
Z. Sheng, J. Zhou, Y. Liu*
10:35 – 833. Carbon nanotube uptake, translocation, and stress effects in corn (*Zea mays* L) grown in soil.
J.E. Canas-Carrell, A.M. Cano, M.M. McManus, S. Deleon, F. Irin, P. Payton, M. Green
10:55 – 834. Exposure of *Arabidopsis thaliana* to iron nanoparticles induces the enhancement of photosynthesis as a result of promoted stomatal opening.
H. Yoon, J. Kim, Y. Kang, Y. Chang*
11:15 Final remarks

Hilton Waikiki Beach
Molokai

Chemistry of Integrated Water Treatment Systems for Halogenated Organics and Long-lived Radionuclides (#454)

Organized by: W. Lee, H. Kim, H. Anderson, M. Diallo, D. Waite
Presiding: W. Lee

8:00 Opening Remark
8:05 – 835. Polymer stabilized nanogold as tracer to use in co-injection with nZVI during in-situ DNAPL remediation.
B. Uthuppu*, A.S. Fjordboege, M. Broholm, M.H. Jakobsen

8:35 – 836. Reductive removal of Cr(VI) using zero-valent magnesium under oxygenated circum-neutral pH conditions.
J. Park, J. Ahn, J. Kim, G. Lee*

9:05 – 837. Microtiter plate based colorimetric assay for characterization of dehalogenation activity of GAC/Fe⁰ composite.
Y. Hwang*, A. Salatas, P.D. Mines, M.H. Jakobsen, H.R. Andersen

9:35 – 838. Uranium immobilization in a contaminated soil column by iron phosphate mineral.
W. Lee*, Y. Sih

10:05 Break
10:15 – 839. Mechanistic understanding of contaminant degradation on the catalyst surface.
H. Kim*, K. Jeon, H. Shin

10:45 – 840. Nanoporous disulfide networks for selective uptake for halogenated organics and ethers. H. Patel, J. Byun, M.S. Yavuz, C.T. Yavuz

11:15 – 841. Covalent organic polymer functionalized activated carbon: A novel material for water contaminant removal and CO₂ capture.
P.D. Mines*, D. Thirion, B. Uthuppu, Y. Hwang, M.H. Jakobsen, H.R. Andersen, C.T. Yavuz

11:35 – 842. Simultaneous determination of heavy metal ions in contaminated groundwater by absorption spectrophotometry with Br-PADAP (2-(5-bromo-2-pyridylazo)-5-diethylaminophenol).
T. Kim*, J. Yun

11:55 Closing Remark

Saturday Afternoon

Hilton Waikiki Beach
Territorial III

Pectin Chemistry and Technology (#20)

Organized by: B. Savary, M. Williams, S. Lu, S. Yoo, R. Cameron

13:00 (delay session start)
13:15 Opening
13:20 – 843. Thermostable pectinases for processing pectin-rich food and agricultural biomass – evaluation for *in planta* expression.
B. Savary*, J.C. Tovar, J. Xu, N. Zhang

13:50 – 844. Directed expression of an endo-arabinanase in plants with a designer molecular carrier and colon-endothelium functioning by arabino-oligosaccharide products.
J. Xu, N. Zhang, B.J. Savary

14:20 – 845. Colon-specific delivery of *Lactobacillus rhamnosus* GG using pectin hydrogel beads.
L. Liu

14:50 Break

15:00 – 846. Encapsulation of a model compound in pectin delays its release from a biobased polymeric material.
V.L. Finkenstadt*

15:30 – 847. Role of bioactive pectic polysaccharides on intestinal immune system.
H. Yamada*, H. Kiyohara

16:00 – 848. Bioactive pectic oligosaccharide structure function relationships.
A. Hotchkiss*

16:30 Closing

Hilton Waikiki Beach
Hawaii

Human Exposure to Environmental Contaminants (#26)

Organized by: J. Martin, K. Kannan, L. Zhu, H. Moon
Presiding: J. Martin, H. Moon

13:00 – 849. Bisphenol A and its replacement BPS induce precocious neurogenesis and hyperactivity in zebrafish.
D. Kurrasch*, C. Kinch, K. Ihazheviebo

13:40 – 850. Maternal co-exposure to methylmercury (MeHg) and perfluorooctane sulfonate (PFOS) alters the neurodevelopment of Sprague-Dawley rat pups.
A. Reardon*, K. Fouad, T. Hamilton, J.P. Benskin, B. Chandramouli, J.R. Cosgrove, E. Khodayari, I. Dinu, J. Martin

14:00 – 851. Polybrominated diphenyl ethers and 2,4,6-tribromophenol and their associations with thyroid hormone levels and thyroid sulfotransferase activity in human placental tissues.
H. Stapleton, C. Leonetti, C. Butt, K. Hoffman, M. Miranda

14:20 – 852. Pesticide residues and dietary risk assessment of pesticides in fruits and vegetables in Beijing, China from 2012 to 2014. n. zou*, c. yu, y. li, Y. Han, y. qin, k. gu, j. zhang, C. Pan*

14:40 – 853. Using chemical and in-vitro cell-based methods for the presicion of bioavailability of arsenic and cadmium in health risk assessment.
J. Ng*, B.N. Noller, C. Peng, V. Diacomanolis, R. Taga, H. Harris, Q. Xia

15:00 – 854. In vitro demonstration of polycyclic aromatic hydrocarbon uptake, biotransformation and DNA-adduct formation in human liver cells.
V. Lal*, C. Peng, M. Fletcher, S. Were, J. Ng

15:20 – 855. Human and environmental risk assessment: A chemical fugacity and activity approach.
F.A. Gobas, D. Mackay, J.A. Arnot

15:40 – 856. Biomonitoring persistent organic pollutants and emerging contaminants in breast milk from Korea.
S. Lee*, s. kim, j. park, H. Kim, J. Lee, G. Choi, S. Choi, S. Kim, S. Kim, s. kim, K. Choi, H. Moon

16:00 – 857. Several persistent environmental chemicals among susceptible human populations, and endocrine disruption: Epidemiological observations and experimental evidences. s. kim, S. Kim, H. Kang, J. Jung, H. Moon, s. kim, j. park, K. Choi*

Hilton Waikiki Beach
Territorial I & II

Recycling of Polymeric Materials: Challenges and Perspectives (#36)

Organized by: T. Yoshioka, K. Joo-Sik, V. Sahajwalla, B. Thallada

13:00 No name

14:00 – 858. Rapid and highly effective conversion of biomass into chemicals and fuels under hydrothermal conditions.
F. Jin*, G. Yao, Z. Huo

14:40 – 859. Biosynthesis of polyhydroxyalcanoates (PHAs) using volatile fatty acids (VFAs) generated from the wastewater sludge of Fe-enhanced primary treatment.
L. Lin*, X. Li, H. Li, J. Xu, R. Li, L. Lin

15:00 – 860. Production of volatile fatty acids (VFAs) from the wastewater sludge of the AI-enhanced primary treatment.
L. Lin*, X. Li, H. Li, J. Xu, R. Li, Y. Li

15:20 – 861. Status and strategies for effective utilization of lignocellulosic biomass in India: Case study. **B. Thallada***

16:00 – 862. Pyrolysis: a promising process for the utilisation of lignocellulosic biomass in decentralised units.
B.B. Krishna, B. Biswas , J. Kumar, R. Singh, B. Thallada*

16:20 – 863. Energy recovery from municipal solid waste incineration in Japan.
M. Takaoka*, T. Yokoyama

Hilton Waikiki Beach
Altitude

Chemical Ecology Applied to Sustainable Agriculture (#105)

Organized by: C. Osorio, J. Bento, T. Ando, X. Chen

Presiding: T. Ando, X. Chen

13:00 Introductory Remarks

13:05 – 864. Aluminum oxalate complex as an antimicrobial substance from the active mycorrhizal zone of *Tricholoma matsutake*. **K. Nishino***, M. Shiro, K. Oizumi, R. Okura, T. Fujita, A. Yamada, C. Tanaka, T. Sasamori, N. Tokitoh, N. Hirai

13:35 – 865. Regulatory factors that control asexual reproduction of the plant pathogen *Phytophthora*. **M. Ojika***, R. Iwai, C. Han

14:05 – 866. Measurements of nitrous acid (HONO) direct emission from rice paddy soil and its contribution to atmospheric HONO. **C. Minejima***, R. Nakane, K. Shimada, S. Riya, K. Sato, M. Ohyama, A. Terada, M. Hosomi

Hilton Waikiki Beach
Kauai

Enzymes Essential to Biosphere Health: Bioremediation and Biogeochemical Cycling (#219)

Organized by: L. Eltis, M. Fukuda, L. Wackett

13:00 – 867. Halokane dehalogenases in bacteria. **Y. Nagata***, R. Moriuchi, Y. Ohtsubo, M. Tsuda

13:25 – 868. New chemistry in biodegradation of (halogenated) aromatic compounds. **D. Ley***

13:50 – 869. Kinetic, mechanistic, and structural characterization of three hydratase/alcoholases in polycyclic aromatic hydrocarbon degradation: Analysis and Implications. **C.P. Whitman***, W.H. Johnson, W. Li, Y. Zhang

14:15 – 870. Bacterial phosphate uptake: Sub-Angstrom insights into exquisite molecular discrimination. R. Qi, A. Wellner, D.S. Tawfik, **m. elias***

* Principle Author

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14:40 – 871. Phosphotriesterases as catalysts for the hydrolysis and detoxification of organophosphate nerve agents.
F.M. Raushel*

15:05 – 872. Formation and breakdown of compounds with phosphorus-carbon bonds. **W.A. van der Donk***

15:30 – 873. Evolutionary contingency in an emergence of an organophosphate hydrolase. **N. Tokuriki***

15:55 – 874. Enzyme engineering for the bioremediation of s-triazine compounds. **L.P. Wackett***

Hilton Waikiki Beach
Molokai

Chemistry of Integrated Water Treatment Systems for Halogenated Organics and Long-lived Radionuclides (#454)

Organized by: W. Lee, H. Kim,
H. Anderson, M. Diallo, D. Waite
Presiding: J. Han

13:00 Opening Remark

13:05 – 875. Mining critical metals and uranium from seawater: Overview of recent advances. **M. Diallo***, M. Kotte, M. Cho

13:35 – 876. Innovative fuel cell-based technologies for the treatment of H₂S and electricity generation. K. Kim, **J. Han***

14:05 – 877. Remediation of pharmaceuticals in DOM containing wastewaters. **T.A. Reutershan**, S. Mezyk

14:35 Break

14:50 – 878. Removing antibiotics from wastewater: Alternative radical treatments. **C.A. Rice**, S. Mezyk

15:20 – 879. Water purification by a novel flow plasma. **Y. Mizukoshi***, H. Horibe, Y. Nishimura

15:50 Closing Remark

Saturday Evening

Hawaii Convention Center
Halls I, II, III

Human Exposure to Environmental Contaminants (#26)

Organized by: J. Martin, K. Kannan,
L. Zhu, H. Moon
Presiding: K. Kannan, J. Martin, H. Moon,
L. zhu

Poster Session

19:00 – 21:00

880. Survey of cyclic and linear siloxanes in indoor dust and their implications for human exposures in twelve countries. T.M. Tran, K. Abualnaja,

A. Asimakopoulos, A. Covaci, B. Gevao, **T.A. Kumosani**, K. kannan*

881. Cyclic and linear siloxanes in indoor air from Albany, New York, USA, and its implications for inhalation exposure. **K. Kannan**, T.M. Tran

882. Parabens and their derivatives in pharmaceuticals: A source of human exposure. **K. Kannan***, C. Moreta, M. Tena

883. Human exposure assessment by characterization of perfluorocarboxylic acids and typical isomers in foodstuff, indoor dust and tap water in Tianjin, China. **L. zhu***

884. Comparative assessment of human exposure to tetrabromobisphenol A and eight bisphenols including bisphenol A via indoor dust ingestion in twelve countries. T.A. Kumosani, W. Wang, **K.O. Abulnaja**, A. Asimakopoulos,

A. Covaci, B. Gevao, B. Johnson-Restrepo, G. Malarvannan, T.B. Minh, H. Moon, H. Nakata, R.K. Sinha, K. kannan*

885. Method for evaluating the exposure concentration of phenols in water. **w. zhong**, d. wang, L. zhu

886. Occurrence of phthalate diesters in particulate and vapor phases in indoor air and implications for human exposure in Albany, New York, USA. **T.M. Tran***, K. Kannan

887. Changes of chemical characteristics of the outdoor, indoor, and individual exposure of suspended particles in Osaka, Japan. **K. Funasaka***

888. Development of suppression method for boron elution from coal ash with formation of insoluble inorganic salt. **N. Sugai**, T. Kawashima, T. Naruse, A. Sasaki, M. Endo

889. Study on the inhibition of dissolution fluoride from the sludge. **X. Kuang**, A. Sasaki, M. Endo

890. Investigating the influence of temperature and acid matrix on the determination of arsenic in the As reference speciation standards. **S. Rabib***, M. Le, L. Yu

891. Association between arsenic concentration and satisfaction level for well water in Basailboogh village, Bangladesh. **M. Sekine***, M. RAKNUZZAMAN, M. Tokumura, K. AHMED, S. Masunaga

892. Study on the exposure by environmental samples for arsenic species using ion chromatography coupled with mass spectrometry. **J. Lee***

893. Physico-chemical and microbiological characteristics of the nearshore and surface sediments environment of the Hawkbill Turtles (Pawikan) Sanctuary in Davao City. **V.C. Badong***

Hawaii Convention Center
Halls I, II, III

Recycling of Polymeric Materials: Challenges and Perspectives (#36)

Organized by: T. Yoshioka, K. Joo-Sik, V. Sahajwalla, B. Thallada

Poster Session

19:00 – 21:00

894. Adhesion behavior of blue mussel (*Mytilus galloprovincialis*) and effects of poly(l-lactic acid). **T. Furukawa**, H. Nishida

895. Preparation of activated carbon from phenol resin for adsorption of low concentration benzene from humid air. **A. Hiwada**, M. Uddin, Y. Kato

896. Effect of reaction environment on hydrothermal valorization of lignin. **A. Prakash**, R. Singh, B.B. Krishna, J. Kumar, B. Thallada*

897. Scrap tire pyrolysis using a two stage pyrolyzer and absorbents for the removal of sulfur in pyrolysis oil and char. **G. Choi***, S. Oh, J. Kim

898. Basic study of advanced material recycle of waste plastics based on the physical degradation theory. **A. Tominaga**, H. Sekiguchi, R. Nakano, S. YAO*, E. Takatori

899. Fluid catalytic cracking reaction of waste plastic: Effect of addition of woody biomass. **K. Otani***, K. Momono, K. Takagi, N. Okazaki

900. Fluid catalytic cracking reaction of waste plastic: Activities of the iron-based catalysts. **T. Hotta***, K. Otani, K. Momono, K. Takagi, N. Okazaki

901. Geopolimerization of pulp paper industrial wastes for thermal insulating application. **M.P. Seabra***, R.M. Novais, L.H. Buruberri, J.A. Labrincha

902. Preparation of quality control plastic disks containing flame retardants and application to the weathering tests. **N. Itoh***, T. Otake, M. Ohata, A. Wada, N. Hanari

903. Surface design by photo-vapor-phase-assisted polymerization. **S. Gomi***, H. Nishida

904. Availability of woody biomass degraded by mushrooms as ingredient of fermented total mixed ration for feeding dairy cattle. **N. Nagatani**, T. Kojima, N. Nishino, K. Tokimoto, S. Nagao, T. Nitoda, H. Kanzaki*

Hawaii Convention Center
Halls I, II, III

Chemistry of Integrated Water Treatment Systems for Halogenated Organics and Long-lived Radionuclides (#454)

Organized by: W. Lee, H. Kim, H. Anderson, M. Diallo, D. Waite

Presiding: H. Kim

Poster Session

19:00 – 21:00

905. Theoretical studies on catalytic properties of Au nanoparticles. **T. Eom***, H. Kim

906. Reduction mechanism of nitrophenol to aminophenol on magnetic (111) surface. **S. Gim**, H. Kim

907. Study on regeneration method of spent activated carbon which adsorbs halogenated organics by using liquefied dimethyl ether gas. **T. Sano***, M. Matsuzawa

Sunday Morning

Hilton Waikiki Beach
Territorial I & II

Pectin Chemistry and Technology (#20)

Organized by: B. Savary, M. Williams, S. Lu, S. Yoo, R. Cameron

8:00 Opening

8:10 – 908. Pectin homogalacturonans:

Microstructural characterization of methyl-esterified domains. **R. Cameron***, Y. Kim, A. Galant, G.a. Luzio, J.T. Tzen

8:40 – 909. Characterization of nanostructure introduced into a model pectic homogalacturonan by pectin methyl esterases and relationship between its structure and functionality of calcium-mediated gel. **Y. Kim***, R. Cameron*, G.a. Luzio, B.J. Savary, M.A. Williams, S. Yoo

9:10 – 910. Processive PME as a fine-structure amplifier for high DM substrates: A tale of two pectins. **B. Williams***, R. Cameron, m. ralef, J. Owen

9:40 – 911. Effect of fine-structure on the long timescale dynamics of pectin gels. **J. Owen***, B. Mansel, B. Williams

10:10 Break

10:20 – 912. Role of pectin on the mechanical properties of hydrated cellulose networks as plant cell wall analogs. **P. Lopez-Sanchez**, D. wang, M. Rincon-Bonilla, J. Stokes, M. Gilley

10:50 – 913. Stability of modified low methoxyl pectin under simulated gastric conditions is greater than commercial low methoxyl pectin. **J. Koh**, L. Wicker, Y. Kim

11:20 – 914. Response surface methodology to explore the effects of polyvalent and monovalent cations on the thermal and gelling properties of low DM pectins. **G.a. Luzio***, R. Niedz

11:50 Close

Hilton Waikiki Beach
Hawaii

Human Exposure to Environmental Contaminants (#26)

Organized by: J. Martin, K. Kannan, L. Zhu, H. Moon

Presiding: J. Martin, L. zhu

8:00 – 915. Strategies based on high resolution mass spectrometry to identify novel per- and polyfluorinated alkyl substances (PFAS) in human serum.

M. Gomez Ramos*, A. Rotander, A. Kärman, L.L. Toms, J. Mueller

8:20 – 916. Distribution of perfluoroalkyl acids and the typical isomers between paired human serum and whole blood samples. **L. zhu**

8:40 – 917. Occupational exposure to perfluoroalkyl acids and the isomers in a fluorochemical manufacturing plant in China: Body burden, intake, and half-lives estimation. **J. Fu**, Y. Gao, **Y. Wang**, a. zhang, **G. Jiang**

9:20 – 918. Assessment of human exposure to airborne particles using simulated lung fluids. **R. Balasubramanian***

9:40 – 919. Effects of size and concentration variance of Ag nanoparticles on their interfacial phenomena in the form of surface tension in pulmonary physiology. **J.J. Bang***, T. Poteat, Z. Hendren

10:00 – 920. Studies on environmental pollutants entering food chain in southwest Louisiana - case study. **J. Sneddon***, C.E. Hardaway

10:20 – 921. Hair mercury level and fish consumption: Perception of mercury risk among general residents in China. **Y. ZHANG**, J. ZHOU

10:40 – 922. Identification of environmental sources of lead exposure in Nunavut (Canada) using stable isotopes analyses. **M. Fillion**, J. Blais*, E. Yumivhoze, M. Nakajima, P. Workman, G. Osborne, H. Chan

Hilton Waikiki Beach
Territorial I & II

Recycling of Polymeric Materials: Challenges and Perspectives (#36)

Organized by: T. Yoshioka, K. Joo-Sik, V. Sahajwalla, B. Thallada

8:00 Opening

9:00 – 923. Interactions between beech wood and polyethylene during co-pyrolysis. **S. Kumagai***, K. Fujita, G. Grause, T. Kameda, T. Yoshioka*

9:40 – 924. Deicer preparation from dolomite and bio-oil from the fast pyrolysis of corn cob. **S. Oh***, J. Kim, G. Choi

10:00 – 925. Physical regeneration method of waste plastics based on physical degradation theory. **S. YAO***, A. Tominaga, N. Takenaka, R. Nakano, H. Sekiguchi

10:20 – 926. Generation behavior of nitrogen compounds during steam pyrolysis of polyimide film using Ni-based catalysts. **T. Hosaka***, S. Kumagai, G. Grause, T. Kameda, T. Yoshioka

10:40 – 927. Recovery of useful resources from waste photovoltaic module by liquefaction of cured EVA. **T. Kamo***, H. Ito

11:20 – 928. Applicability of polyurethane foam generated from WEEE as energy sources by thermal methods. S. Park, J. Lee, W. Yang, C. Oh, **Y. Seo***

Hilton Waikiki Beach
Kauai

Enzymes Essential to Biosphere Health: Bioremediation and Biogeochemical Cycling (#219)

Organized by: L. Eltis, M. Fukuda, L. Wackett

8:00 – 929. Structure of anaerobic methane-oxidizing enzyme. **S. Shimai***

8:25 – 930. Making diesel fuel in bacteria via the cryptically-redox oxygenation reaction of aldehyde deformylating oxygenase. **J.M. Bollinger**, M. Pandelia, N. Li, D.M. Warui, W. Chang, H. Norgaard, L.J. Rajakovich, A.L. Compton, C. Krebs, S.J. Booker

8:50 – 931. Emergence of bacterial ligninases. **R. Singh**

9:15 – 932. Catalytic function of aromatic ring-hydroxylating dioxygenase, carbazole 1,9a-dioxygenase. **H. Nojiri***

9:40 – 933. Structure and function of type II extradiol dioxygenases in a catabolic pathway of lignin-derived aromatic compounds. **T. Senda***, K. Sugimoto, M. Senda, D. Kasai, M. Fukuda, E. Masai

* Principle Author

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- 10:05 – 934.** C-C bond-cleaving amidohydrolases involved in biomass degradation. **L. Eltis**, E. Kuatsjaj, H. Otani
- 10:30 – 935.** Enzymes involved in microbial metabolism of toxic compounds and their application. **M. Kobayashi***
- 10:55 – 936.** Rapid oxidation and slow mineralization of iron by a diatom ferritin. S. Pfaffen, J.M. Bradley, G.R. Moore, N.E. Le Brun, **M.E. Murphy**
- 11:20 – 937.** Characterizing Mn²⁺-oxidizing multicopper oxidase complex from *Bacillus* sp. PL-12. **C. Romano***, M. Zhou, L. Tao, T. Stich, Y. Song, C. Butterfield, A. Dohnalkova, L. Paša-Tolić, A. Soldatova, Z. Pinder, W.H. Casey, V. Wysocki, R. Britt, T. Spiro, B. Tebo

BIOL**Area 7 – Biological****Tuesday Morning**

Sheraton Waikiki
Ewa

Low-Energy Photoexcited States in Photosynthesis (#117)

Organized by: J. Reimers, E. Krausz, A. Freiberg, D. Bruce, A. Holzwarth, H. Hashimoto, D. Coker
Presiding: E. Krausz

- 8:00 – 1.** Algae switch excitons on and off in light harvesting. **G. Scholes***
- 8:30 – 2.** Low-energy photoexcited states in Photosystem II: A 2D electronic spectroscopy study. **E. Romero***, V. Novoderezhkin, R. van Grondelle
- 9:00 – 3.** Modeling exciton dynamics and charge transfer states. **T. Kramer***
- 9:30 Break**
- 9:45 – 4.** Low energy coherent oscillations in the non-adiabatic excited state of light-harvesting phycocyanin-645. **J. Davis***, F. Novelli, A. Rozbeh, P. Curmi, K. Wilk
- 10:15 – 5.** Tracking the energy flow through the entire photosynthetic apparatus in situ. J. Dostal, J. Psencík, **D. Zigmantas***
- 10:45 Break**
- 11:00 – 6.** Influence of heterogenous chromophore environments on excitation energy transport in photosynthetic complexes. **D.F. Coker**, M. Lee, D. Montemayor, E. Rivera, S. Jang
- 11:30 – 7.** Quantum coherence between B800 and B850 assemblies of light-harvesting complex from purple bacteria observed by 5 fs optical pulses. **H. Hashimoto***

Royal Hawaiian
Regency III

Advances in Biological Solid-State NMR (#120)

- Organized by: A. Naito, M. Auger, A. Ramamoorthy, F. Separovic, T. Fujiwara, Y. Kim
Presiding: A. Naito, F. Separovic
- 8:00 Opening Remarks**
- 8:10 – 8.** Warburg metabolism in three rapidly proliferating cell lines using solid-state NMR. **J. Schaefer***
- 8:35 – 9.** Aggregation of β -amyloid peptides in confined space. **J.C. Chan***
- 9:00 – 10.** Solid-state NMR of viral fusion proteins. **D. Weliky***
- 9:25 – 11.** MAS NMR of HIV-1 capsid assemblies and their complexes with host factors: Insights into structure and dynamics. M. Lu, G. Hou, M. Wu, C. Suiter, H. Zhang, R. Gupta, C. Quinn, X. Lu, J. Ahn, I. Byeon, C. Aiken, P. Zhang, J. Perilla, K. Schulter, A.M. Gronenborn, **T. Polenova***
- 9:50 Break**

- 10:05 – 12.** Molecular complexity of sea silk as revealed by solid-state NMR. A.A. Arnold, B. Genard, F. Byette, C. Pellerin, R. Tremblay, **I. Marcotte***
- 10:30 – 13.** Structure and propagation of amyloid fibril for 42-residue amyloid- β A β (1-42) and nano-mole-scale protein solid-state NMR using ultrafast MAS. **Y. Ishii**
- 10:55 – 14.** Spectral snapshots of bacterial cell-wall composition and the influence of antibiotics by whole-cell NMR. J. Romaniuk, R. Nygaard, D. Rice, **L. Cegelski**
- 11:20 – 15.** NMR characterization of conformational transition of amyloid- β peptide promoted on ganglioside clusters. M. Yagi-Utsuri*, **K. Nishimura**, K. Kato*
- 11:35 – 16.** Amyloid, membranes, micro-waves, and the magic angle. **R. Griffin***

Sheraton Waikiki
Kohala/Kona

Fluorescent and Luminescent Proteins: New Chemistries and New Functions (#180)

Organized by: M. Lin, R. Campbell, T. Nagai

- 8:00 Miyawaki**
- 8:30 – 17.** Physical bases for developing next generation far red fluorescent proteins. **H. Ng***
- 9:00 – 18.** Far-red fluorescent protein evolved from the phycobilisome of a cyanobacteria. **E.A. Rodriguez**, G.N. Tran, R.Y. Tsien
- 9:30 – 19.** Capturing photoinduced structural snapshots of emerging fluorescent protein biosensors with ultrafast vibrational spectroscopy. W. Liu, B.G. Oscar, L. Tang, Y. Wang, Y. Zhao, R.E. Campbell, **C. Fang***
- 10:00 – 20.** Computational exploration of one- and two-photon absorption in fluorescent protein chromophores. **A. Brown***, M.A. Salem
- 10:15 – 21.** Multicolor monomeric near-infrared fluorescent proteins engineered from bacterial phytochromes. **D.M. Shcherbakova**, M. Baloban, **V.V. Verkhusha***
- 10:45 – 22.** Developing photoactivatable fluorescent proteins for super-resolution imaging. **P. Xu**
- 11:15 Zhang**
- 11:45 – 23.** Improving optical control of protein activities with an engineered photodissociable dimeric fluorescent protein domains. **M. Lin**

Royal Hawaiian
Regency I

Frontiers of Iron Chemistry in Biology (#268)

Organized by: K. Ishimori, S. Sliger, G. Mauk
Presiding: A.G. Mauk, J.S. Olson, E. Raven

- 8:00 – 24.** Structural and functional characterization of heme-regulated proteins: Heme as a signaling molecule. **K. Ishimori***
- 8:24 – 25.** Probing [4Fe-4S] and nitrosyl chemistry with NRVS, Mössbauer, and EXAFS, for WhiD and NsrR proteins. **P. Serrano***, H. Wang, S. George, S. Kamali, J.C. Crack, M. Hu, E.E. Alp, N.E. Le Brun, S. Cramer
- 8:43 – 26.** Heme modulates cardiac K_{ATP} channel function. **E. Raven**
- 9:07 – 27.** Hydrogen bonding interactions in ligand sensing and signaling by *Mycobacterium tuberculosis* DosS and DosT. Y. Madrona, D. Basudhar, S. Sivaramakrishnan, E. Yukl, P. Moënne-Loccoz, **P.R. Ortiz de Montellano***
- 9:31 – 28.** Ligand discrimination by hemoglobins and myoglobin: How does it work and why should we care?. **J.S. Olson***
- 9:55 – 29.** New twist on heme structure and function. **K.L. Bren***

- 10:19 – 30.** Human indoleamine 2,3-dioxygenase isoforms IDO1 and IDO2: A study in contrasts. H.H. Kuo, **G. Mauk***
- 10:43 Break**
- 10:53 – 31.** Determination of the iron(IV/III) reduction potential in P450 compound II. **M. Green**

11:17 – 32. Oxygen activation by cytochrome P450. **S.G. Sligar**

11:41 – 33. Making and breaking heme in *Staphylococcus aureus*: New enzymological developments. **J. DuBois***, B. Streit

Sheraton Waikiki
Kahuku

Chemical Approaches to Astrobiology (#326)

Organized by: H. Mita, H. Cleves, A. Negron-Mendoza, H. Yabuta
Presiding: H. Mita, A. Negron-Mendoza, H. Yabuta

8:00 Introductory Remarks

8:05 – 34. Identity as life acquired by hierarchical dynamics emerged in molecular system. **T. Sugawara***

8:35 – 35. Theoretical and methodological issues in the study of the origin of life. **A. Lazcano***

9:05 – 36. Purine biosynthetic intermediate-containing ribose-phosphate polymers as evolutionary precursors to RNA. **H.S. Bernhardt***, R. Sandwick

9:25 – 37. Simplification of the genetic code: Restricted diversity of genetically encoded amino acids. **D. Kiga***, K. Amikura

9:45 – 38. Drawbacks regarding the chemical evolution of biopolymers under the primitive hydrothermal earth environments. **K. Kawamura***

10:05 Break

10:20 – 39. Nature of the Last Common Ancestor and early evolution of autotrophy. **A. Becerra***

10:40 – 40. CHIRGEN approach to decipher the possible origin of genetic asymmetry.

T. Buñue, G. Cocho, H.I. Cruz-Rosas, L. Le Sergeant d'Hendecourt, P. de Marcellus, U.J. Meierhenrich, C. Meinert, I. Mygorodskaya, L. Nahon, A. Negron-Mendoza, L. Rendon, P. Santiago

11:00 – 41. Size, shape, functional group distributions of organic microspheres formed by Maillard-type reaction. **A. Takahashi**, H. Yabuta

11:20 – 42. Abiotic origins of fundamental metabolic pathways from amino- and α -keto acids. **G. Springsteen**

11:40 – 43. Prebiotic polyamino acid formation under molten states. **H. Mita***, E. Nagasawa, S. Nomoto

Sheraton Waikiki
Honolulu

Chemical Biology of Protein-Lipid Modification (#421)

Organized by: M. Distefano, J. Ohkanda, Y. Chen
Presiding: J. Ohkanda

8:00 – 44. Investigating RAS GTPases' lipid modifications. **Y. Chen***

8:40 – 45. Chemical reporters for exploring protein fatty-acylation. **H. Hang***

9:20 – 46. Imaging cellular protein fatty acylation. **R. Hannoush***

10:00 Break

10:20 – 47. Development of stably membrane-anchoring molecules for "chemical transformation" of cells. **T. Mori***, W. Hatanaka, M. Takeo, R. Tokunaga, M. Kawaguchi, A. Kishimura, Y. Katayama

11:00 – 48. Elucidation of the isoprenylated substrate binding site in ras carboxyl methyltransferase using biotinylated photofrin probes. A. Funk, K. Hahne, J. Verwacke, L. Shrestha, J.L. Donelson, R.A. Gibbs, M. Distefano, **C. Hrycyna***

11:40 – 49. Development and application of small molecule probes for the analysis of protein prenylation. **M. Distefano**

Tuesday Afternoon

Sheraton Waikiki
Ewa

Low-Energy Photoexcited States in Photosynthesis (#117)

Organized by: J. Reimers, E. Krausz, A. Freiberg, D. Bruce, A. Holzwarth, H. Hashimoto, D. Coker
Presiding: D.F. Coker

13:00 – 50. Elucidation of the mechanisms of photoprotection in single LHClI complexes. **G. Schlau-Cohen***

13:30 – 51. Making every photon count: Single molecule spectroscopy applied to natural light-harvesting materials. **r. van grondelle***, T.P. Krüger

14:00 – 52. Explicit calculation of coupled excited states in photosystems. **T.J. Frankcombe***

14:30 Afternoon tea

14:45 – 53. Assignments of the lowest excited states of CP43, CP47 and Photosystem II core complexes via the new technique of temperature dependent circular polarization of luminescence. **E. Krausz***, J. Hall, R. Picolt, J. Shen

15:15 – 54. On the excited state electronic structure, excitation energy transfer, and electron-phonon coupling in selected photosynthetic antenna protein complexes. **R. Jankowiak***, J. Chen, M. Jassas, A. Kell

Royal Hawaiian
Regency III

Advances in Biological Solid-State NMR (#120)

Organized by: A. Naito, M. Auger, A. Ramamoorthy, F. Separovic, T. Fujiwara, Y. Kim
Presiding: T. Fujiwara, I. Marcotte

13:00 – 55. Dynamic nuclear polarization at 16.4 T and 30 K using a novel closed-cycle helium-cooling MAS NMR probe system. **Y. Matsuki**, T. Idehara, Y. Tatematsu, J. Sirigiri, S. Nakamura, T. Fujiwara

13:25 – 56. NMR determination of C-H-N distances for unlabeled molecules. **j. Amoureaux***

13:40 – 57. Single crystal NMR of magnetically oriented microcrystal array. **R. Kusumi**, F. KIMURA, T. Kimura

13:55 – 58. Overtone ¹⁴N solid-state NMR: A route to natural abundance C-N correlations. **L. O'Dell***

14:20 – 59. Photoactivation pathways of photoreceptor membrane proteins revealed by in-situ photo-irradiation solid-state NMR. **A. Naito***

14:45 Break

15:00 – 60. Instrumentation development for 2H NMR of biological solids. **R.W. Martin***

15:25 – 61. Recent advances in ¹⁷O NMR spectroscopy of biological solids. **G. Wu**

15:50 – 62. Using liquids to probe solids with NMR diffusometry. **W.S. Price***, G.R. Dennis, B. Ghadirian, T. Stait-Gardner, A.M. Torres, S.A. Willis, G. Zheng

*** Principle Author**

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214–TECH

16:15 – 63. Short- and long-distance spin-spin correlations for spectroscopic assignment and distance information in solid-state NMR of macroscopically aligned membrane proteins. **A. Nevzorov**
16:30 – 64. 1020 MHz LTS/HTS NMR: Application to solid-state NMR. **Y. Nishiyama**
16:45 – 65. Closed-loop MAS-DNP-NMR at 30 K for affordable dramatic gains in S/N. **J. Staab, J. Spitzmesser, D. Arcos, J. Doty, V. Cothran, M. Bremmer, G. Doty, D. McMee, H. suematsu, L. Holte, P. Ellis, F. Doty**

Sheraton Waikiki
Kohala/Kona

Fluorescent and Luminescent Proteins: New Chemistries and New Functions (#180)

Organized by: M. Lin, R. Campbell, T. Nagai
13:00 – 66. Fluorescent protein-based redox probes. **H. Ai**
13:30 – 67. Directed evolution and structure-guided recombination of fluorescent membrane proteins. **F.H. Arnold***
14:00 – 68. mGRASP for mapping mammalian synaptic circuit at multiple scales. **J. Kim**
14:30 – 69. Directed evolution via multiparameter microfluidic screening to identify new red fluorescent proteins with longer lifetimes and higher photostability. **F. Vietmeyer, K. Dean, P. Manna, P. Friis, L. Davis, R. Jimenez, A.E. Palmer**
14:45 – 70. FRET imaging in organoids and mice. **E. Kiyokawa***
15:15 – 71. Bioimaging with bright luminescent proteins: Comparing pros and cons of fluorescence and luminescence. **T. Nagai***

Royal Hawaiian
Regency I

Frontiers of Iron Chemistry in Biology (#268)

Organized by: K. Ishimori, S. Sliger, G. Mauk
Presiding: B.M. Hoffman, K. Ishimori, J.D. Lipscomb
13:00 – 72. Heme regulates protein-protein interaction of transcription factor Bach2. **M. Matsui, T. Matsui, M. Ikeda-Saito, K. Igarashi, K. Murayama***
13:19 – 73. Crystal structure of HydG and [FeFe] hydrogenase H-cluster biosynthesis. **P.L. Roach**
13:38 – 74. Diversity of the heme-copper oxidoreductase superfamily. **J. Hemp, R. Murali, R.B. Dennis***
14:02 – 75. Visualizing oxygen activation in mononuclear nonheme iron oxygenases. **C.J. Knot, B.S. Rivard, M.S. Rogers, J.D. Lipscomb***
14:26 break
14:36 – 76. New synthetic approaches to heme-O₂-copper assemblies and insights into the O-O reductive cleavage using proton-electron sources. **K.D. Karlin***
15:00 – 77. Fungal tyrosinase. Crystal structures and maturation process. **S. Itoh*, N. Fujieda**
15:24 – 78. Structure, dynamics, and mechanisms of zinc and iron receptors which regulate gene expression. **T.V. O'Halloran**
15:48 – 79. Biosynthesis of the catalytic H-cluster of [FeFe] hydrogenase. **R. Britt***
16:12 – 80. X-ray spectroscopy combined with crystallography for studying water oxidation reaction in Photosystem II at XFEL. **J. Yano*, J. Kern, V. Yachandra, R. Chatterjee, F. Fuller, S. Gul, U. Bergmann, R. Alonso-Mori**
16:36 – 81. Why nature uses radical SAM enzymes so widely: ENDOR studies of lysine 2,3-aminomutase shows the 5'-dAdo[•] 'free radical' is never free. **B.M. Hoffman*, M. Horitani, A. Byer, K.A. Shisler, T. Chandra, J.B. Broderick**

Sheraton Waikiki
Kahuku

Chemical Approaches to Astrobiology (#326)

Organized by: H. Mita, H. Clerves, A. Negron-Mendoza, H. Yabuta
Presiding: H. Mita, A. Negron-Mendoza, H. Yabuta

13:00 – 82. Approaches to structural complexity analysis in abiotic planetary organics. **M.A. Smith*, H. Imanaka**
13:30 – 83. Organic chemistry in planetary atmospheres: Chemical potential toward the origins of life. **H. Imanaka***, M.A. Smith

14:00 – 84. 1D photochemical model coupled to chemical disequilibrium applied to Archean atmospheres. **S.O. Danielache**
14:20 – 85. Evidence from meteorites for multiple amino acid alphabets for the origins of life. **A. Burton*, J.E. Elsila, M.P. Callahan, O.P. Glavin, J.P. Dworkin**
14:40 – 86. Physical properties of possible glycine precursor, CH₂NH sources. **T. Suzuki, M. Ohishi, T. Hirota, M. Saito**

15:00 Break
15:15 – 87. Solution plasma synthesis of ammonium ions from water-CO₂-N₂ system and its time-resolved spectroscopic study. **H. Yu***, K. Kanno, Y. Hagiwara, M. Banno

15:35 – 88. High power laser-shock experiment of chondritic meteorites: Contributions of hydrocarbons and sulfur-bearing compounds to the early Earth atmosphere. **H. Yabuta***, T. Sakaiya, T. Kondo, S. Ohno, T. Kadono, K. Shigemori, Y. Hironaka, T. Yamanaka
15:50 – 89. Radiation chemical processes in prebiotic chemistry. **A. Negron-Mendoza***, S. Ramos-Bernal, M. Collin-Garcia, A. Heredia

16:10 – 90. Expanding the glyoxylate/dihydroxyfumarate scenario: Production of glyceric acid and other aldonic acids. **C.J. Butch*, R. Vindas, J.D. Crowe, P.L. Pollet, R. Krishnamurthy, C.L. Liotta**

16:30 – 91. Chemical astrobiology experiments in Earth orbit: The Tanpopo Mission and beyond. **K. Kobayashi***, Y. Kubekawa, H. Mita, Y. Bessho, H. Yabuta, H. Shibata, J. Takahashi, K. Nakagawa, E. Imai, Y. Ishibashi, K. Okudaira, H. Yano, H. Hashimoto, S. Yokobori, A. Yamagishi

16:45 – 92. Using experimental evolution to assess a possible early origin for DNA. **A. M. Poole**

Sheraton Waikiki
Honolulu

Chemical Biology of Protein-Lipid Modification (#421)

Organized by: M. Distefano, J. Ohkanda, Y. Chen
Presiding: Y. Chen

13:00 – 93. Structure-based design of PPI inhibitors that disrupt ras prenylation. **J. Ohkanda***

13:40 – 94. Protein farnesylyltransferase inhibitors: From oncology to progeria. **C. Strickland***

14:20 – 95. Signaling pathways that regulate the prenylation of small GTPases in cancer. **C. Williams***

15:00 Break
15:20 – 96. Postsynaptic nanodomain regulated by PSD-95 palmitoylation machinery. **M. Fukata***, Y. Fukata

16:00 – 97. Membrane composition and protein lipidation as determinants of the free energy of HIV-1 matrix protein membrane binding. **M. Barros, F. Heinrich, S. Datta, A. Rein, H. Nanda, M. Löschke**

Wednesday Morning

Sheraton Waikiki
Ewa

Low-Energy Photoexcited States in Photosynthesis (#117)

Organized by: J. Reimers, E. Kraus, A. Freiberg, D. Bruce, A. Holzwarth, H. Hashimoto, D. Coker
Presiding: T. Renger

8:00 – 98. Rebuilding the photosynthetic unit: Moving energy in, and electrons out, of the reaction center in nanoscale model systems. **N. Woodbury***, D. Seo, T. Beatty, S. Lin, H. Yan, A. Carey, S. Levenberg, P. Dutta, R. Yang, M. Liu, T. Murrell, H. Zhang, D. Mieritz, K. Jeon, D. Jun, R. Saer, d. matyushov, D. Martin

8:30 – 99. Simulation of electronic spectra line-shapes of chlorophylls in different environmental conditions. **M. Biczysko***

9:00 – 100. Structure-based identification of low-energy excited states in photosynthetic antenna complexes: Electrostatics and beyond. **F. Mühl***
9:30 morning tea

9:45 – 101. Photosynthetic complexes studied with picosecond spectroscopy: From dead crystals to living cells. **H. van Amerongen**

10:15 – 102. Far-red light induced photosynthesis. **F. Mamedov***, J. Jacques, A. Thapper, F. Movkist, S. Styring

10:45 break

11:00 – 103. Linear and non-linear excitation of low-energy excited states in photosynthetic systems and related pigments. **P.J. Walla**

11:30 – 104. Energy transfer dynamics in pigment-protein complexes. **M. Lee, D.F. Coker**

Royal Hawaiian
Regency III

Advances in Biological Solid-State NMR (#120)

Organized by: A. Naito, M. Auger, A. Ramamoorthy, F. Separovic, T. Fujiwara, Y. Kim
Presiding: Y. KIM, A. Ramamoorthy

8:00 Introductory Remarks

8:15 – 105. Structure and dynamics of G protein-coupled receptors and interactions with their ligands in phospholipid bilayers. **S. Park***, A. De Angelis, B. Das, H. Pavlova, J. Radoicic, S. Berkamp, V.S. Wang, Z. Long, S.J. Opella

8:40 – 106. NMR and EPR structural studies of membrane proteins. **G.A. Lorigan***

9:05 – 107. Backbone structure determination of protein in solid-state using paramagnetic relaxation enhancement and chemical shifts. **M. Demura**

9:30 – 108. Structural characterization of fully protonated proteins by ultrafast MAS. **R.J. Linser***, S. Vasa, P. Rovo, K. Grohe, S. Xiang, N. Kulminskaya

9:45 – 109. Advancing structure determination of membrane proteins in lipid bilayer membranes. **F.M. Marassi***

10:00 Break

10:15 – 110. Solid-state NMR characterization of a panel of membrane proteins in phospholipid bilayers. **S.J. Opella***

10:40 – 111. Solid-state NMR analysis of proteins by spectral simulation. **T. Fujiwara***

11:05 – 112. Inactivation of a potassium channel. **A. McDermott*, I.V. Sergeyev**

11:30 – 113. Structure and dynamics of Anabaena Sensory Rhodopsin studied by magic angle spinning solid-state NMR. **V. Ladizhansky**

Sheraton Waikiki
Kauai

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

Organized by: Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang
Presiding: Y. Zheng

8:00 – 114. Discovery of chemical probes for histone methyltransferases. **J. Jin**

8:30 – 115. Journey of developing chemical tools to interrogate protein methyltransferases. **M. Luo**

9:00 – 116. Synthesis of cyclodepsipeptide histone deacetylase inhibitors. **T. Doi***

9:30 – 117. Mechanism-based inhibition of protein N-terminal methyltransferase. **R. Huang**

10:00 Break

10:10 – 118. Picking the PADlock: Chemical probes to study the protein arginine deminases. **P.R. Thompson***

10:40 – 119. Discovery of histone lysine demethylase-selective inhibitors. **T. Suzuki***

11:10 – 120. Novel eight-membered products from polyamines under oxidative stress conditions: Possible epigenetics modulators. **K. Tanaka***

11:40 – 121. Exploring chemical strategies to control and analyze protein methylations. **Y. SOHTOME**, J. Barjau, S. Fujishiro, K. Dodo, A. Ito, M. Yoshida, T. Shimazu, Y. Shinkai, M. Sodeoka*

Hawaii Convention Center
Halls I, II, III

Fluorescent and Luminescent Proteins: New Chemistries and New Functions (#180)

Organized by: M. Lin, R. Campbell, T. Nagai

Poster Session

10:00 – 12:00

122. Novel bright large-Stokes shift fluorescent protein improves the sensitivity of dual-emission microscopy and deep-tissue imaging. **J. Chu*, M. Lin**

123. Development of intrabody-based FRET probe for monitoring histone H3 acetylation in living cells. **C. Chung, Y. Ohmuro-Matsuyama, Y. Sato, H. Kimura, H. Ueda**

124. Optical control of extending neurite direction with light-induced protein oligomerizing system. **M. Endo, M. Hattori, T. Ozawa***

125. Visible-wavelength two-photon excitation of fluorescent proteins for multicolor and high-resolution imaging. **K. Fujita***, M. Yamanaka, K. Saito, N.I. Smith, Y. Arai, K. Uegaki, Y. Yonemaru, K. Mochizuki, S. Kawata, T. Nagai

126. QM/MM free energy perturbation calculations to probe the formation of an active photoprotein. **T.M. Griffiths***, A. Oakley, H. Yu

127. Novel genetically encoded antibody-based biosensor for fluorescence ratio detection of antigen. **K.P. Huynh Nhat, T. Watanabe, T. Hohsaka***

128. Engineering light inducible proteins to control biomolecule activity and behavior in live cells. **Z. Huang, Y. Wang**

* Principle Author

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129. Genetically-encoded chemiluminescent indicator applicable in millisecond voltage phenomena. **S. Inagaki**, T. Matsuda, Y. Arai, Y. Jinno, H. Tsutsui, Y. Okamura, T. Nagai*

130. HIV-1 Rev or Tat fused fluorescent proteins induces its folding and emission by binding with corresponding RNAs. **Y. Itou**, K. Takahashi, T. Tanaka, S. Urata, H. Kozuka, A. Kikuchi, K. Hamasaki*

131. Quenching-type of fluorescent Ca^{2+} indicator for detecting neuronal inhibition. **S. Kuge**, T. Nishihara, T. Matsuda, H. Furukawa, T. Teramoto, T. Nagai, T. Ishihara

132. Intravital two photon imaging with integrated use of chemical probes, dyes, and fluorescent proteins in living animals. **S. Nishimura***

133. Chiroptical properties of fluorescent protein UnaG. **Y. SHITASHIMA***, T. SHIMOZAWA, M. ISHIDA, T. ASAHI

134. Multiple color palette of super-duper luminescent proteins for long-term and ultrafast acquisition of biological phenomena. **K. Suzuki**, K. Enami, S. Mizobuchi, Y. Arai, M. Nakano, T. Nagai*

135. Development of a genetically-encoded probe to visualize β -actin mRNA in living cells based on a reconstituted GFP and an RNA binding domain PUM-HD. **H. Yoshimura**, T. Yamada, T. Ozawa*

Sheraton Waikiki
Maui

Strategies for Coupling and Decoupling Diverse Molecular Units in the Glycosciences (#201)

Organized by: Z. Witzczak, M. Brimble, Y. Miura, R. Bielski
Presiding: R. Bielski, Z. Witzczak

8:00 Oppening Remarks

8:05 – 136. Synthesis and application of neoglycopeptides using click chemistry combined with native chemical ligation and enzymatic glycosylation. **M.A. Brimble**

8:40 – 137. Synthetic antitumor vaccines through coupling of mucin glycopptide antigens to proteins. **H. Kunz***

9:15 – 138. NKT cell-dependent glycolipid-peptide vaccines with potent anti-tumour activity. **C. Hayman**, R. Anderson, B. Compton, C. Tang, A. Author-Hall, R. Kowalczyk, M.A. Brimble, D. Larsen, O. Gasser, R. Weinkove, I. Hermans*, G. Painter*

9:50 Break

10:05 – 139. Chemical synthesis of homogeneous glycoproteins and an insight into the relationship between glycosylation pattern and biological activity. **Y. Kajihara***

10:40 – 140. Neoglycopeptides and neoglycoproteins as diagnostic tools and potential vaccines. **K. Michael***, N.S. Schocker, R.A. Ashmus, S. Portillo, I.C. Almeida

11:15 – 141. Coupling polyphenols with carbohydrates, a strategy toward molecules for the prevention of diabetes and Alzheimer's disease. **A.P. Rauter***

11:50 Concluding Remarks

Sheraton Waikiki
Molokai

Physiology and Metabolism of Extremophiles (#249)

Organized by: H. Atomi, J. Reeve, M. Ito, S. Kang
Presiding: S. Kang

8:00 Opening remarks

8:05 – 142. Novel pathway for cysteine biosynthesis in *Thermococcus kodakarensis*. **H. Atomi**, Y. Makino, H. Kawamura, T. Imanaka, T. Sato

8:25 – 143. Structural investigations into a promiscuous metabolic pathway in the Archaeon Sulfolobus solfataricus. **S.D. Bull**, M. Danson

8:50 – 144. Potential of extremophiles for cost-competitive bioenergy production. **L. Christopher***

9:15 – 145. Enhancing cell-specific H_2 production of the hyperthermophilic archaeon *Thermococcus kodakarensis* via genetic engineering. **J.R. Simons**, T. Kanai, H. Atomi

9:35 – 146. Unique property of acetic acid bacteria conferred by a specific regional deletion in a leucine responsive regulator. **Y. Ishii**, N. Akasaka, H. Sakoda, S. Fujwara

9:55 – 147. Cysteine desulfurase, a key enzyme for thriving outside sulfatitic environment in a hyperthermophilic archaeon, *Thermococcus kodakarensis*. **R. Hidese**, S. Fujwara*, T. Imanaka

10:15 Break

10:25 – 148. Physiology and motility of alkaliphilic *bacillus*. **M. Ito***

10:50 – 149. Tactic responses of extremely halophilic archaeon *Halocarcula japonica* overexpressing its aerotaxis transducers. **T. Matsubara**, T. Tadikara, R. Yatsunami, T. Fukui, S. Nakamura*

11:10 – 150. Detection of rotation of archaeal flagella under advanced optical microscopes. Y. Kinoshita, D. Nakane, T. Nishizaka*

11:35 – 151. Multi-omics analysis revealed the mechanism of the degradation of poultry feathers by the extremophilic eubacterium *Fervidobacterium islandicum* AW-1. Y. Lee, K. Chandrasekhar, J. Shin, D. Lee*

Royal Hawaiian
Regency I

Frontiers of Iron Chemistry in Biology (#268)

Organized by: K. Ishimori, S. Sliger,
G. Mauk
Presiding: Y. Shiro, A. Wilks

8:00 – 152. Peroxidase proton coupled electron transfer. **T. Poulos**

8:24 – 153. It makes NO sense: Visualizing nitric oxide receptor gymnastics at ultra-high-resolution. **C.S. Raman***

8:48 – 154. Proton transfer in bacterial nitric oxide reductases coupled with NO reduction. **Y. Shiro**, T. Tosha

9:12 – 155. Biosynthetic models of heteronuclear metalloenzymes involved in multi-electron redox processes. **Y. Lu***, Y. Yu, A. Bhagi-Damodaran, I. Petrik, A. Mukherjee, C. Cui, S. Chakraborty, J. Reed

9:36 break

9:46 – 156. CO releasing proteins as bioinorganic tools for CO gas biology. **T. Ueno***

10:10 – 157. Structural snapshots into mycobacterial heme uptake. N. Chim, R. Morse, A. Chao, G. Batot, C. Goulding*

10:34 – 158. Iron release from heme by Isld and the reductase IruO. S.A. Loutet, S.J. Takayama, M.J. Kobylarz, A.G. Mauk, **M.E. Murphy***

10:58 – 159. Host-pathogen interaction:

Overcoming iron limitation through heme acquisition. **A. Wilks**

11:22 – 160. Paradigm shift in heme degradation. **M. Ikeda-Saito***, T. Matsui, S. Nambu, H. Fujii, S. Takahashi

Hawaii Convention Center
Halls I, II, III

Chemical Approaches to Astrobiology (#326)

Organized by: H. Mita, H. Clerves,
A. Negron-Mendoza, H. Yabuta
Presiding: H. Mita, A. Negron-Mendoza,
H. Yabuta

Poster Session

10:00 – 12:00

161. Origin of terrestrial bioorganic homochirality relevance to asymmetry of the universe: Approaches with synergy effects of observations, experiments, and computations. **J. Takahashi***, M. Tamura, M. Kato, K. Kobayashi, M. Umemura, J. Kwon, N. Kusakabe, M. Hosaka, N. Yamamoto, T. Konomi, K. Matsuo, Y. Ueno, Y. Kamei, M. Ehara, R. Fukuda, K. Shiraishi, H. Shinjojima

162. Formation of complex amino acid precursors from possible interstellar media by particles irradiation. **T. Matsuda***, S. Enomoto, Y. Kebukawa, T. Kaneko, H. Fukuda, Y. Oguri, S. Yoshida, K. Kobayashi

163. Laboratory synthesis of alkyl phosphates in astrochemical ice analogs. **A. Turner***, R. Kaiser, M.J. Abplanalp

164. Mass spectrometric studies of organics in the interstellar ice analogs. **M. Nakayama***, Y. Ishibashi, H. Mita, H. Naraoka, S. Tachibana, T. Hama, Y. Endo, A. Kouchi

165. Organic compounds exposure experiments on the Japanese Experiment Module, the International Space Station. **H. Mita***, K. Kobayashi, K. Nakagawa, H. Yabuta, Y. Kebukawa, E. Imai, Y. Kawaguchi, H. Hashimoto, S. Yokobori, H. Yano, K. Okudaira, M. Tabata, H. Kawai, A. Yamagishi

166. Structure analysis of coolgomers in thermal proteinoids. **E. Nagasawa**, H. Mita

167. Prediction of 66.7% glycerol solution behavior in Mars exploration mission. **M. Nishizawa***, S. Sasaki, E. Imai, T. Sato, A. Yamagishi

168. Thermodynamics and the possibility of life on extra-terrestrial worlds. **N.V. Pandey***

169. Detection of biological activities in extreme environments by amino acid analysis and phosphatase assay. **Y. Ishikawa***, K. Aoki, Y. Obayashi, Y. Kebukawa, T. Kaneko, H. Mita, M. Ogawa, R. Navarro-Gonzalez, K. Kobayashi

Sheraton Waikiki
Lanai

Carbohydrate Recognition in Health and Disease (#342)

Organized by: G. Boons, Y. Ito,
A. Demchenko, D. Vocadlo

8:00 – 170. Glycocalyx engineering toward probing cancer glycome evolution. **C.R. Bertozzi**

8:30 – 171. Carbohydrate HIV vaccine design through directed evolution. **I.J. Krauss**

9:00 – 172. Glycans, guts, and PULs: Carbohydrate recognition in dietary fiber utilization. **H. Brumer***

9:30 – 173. Expanding glycoconjugate library on DNAs and its enhanced affinity to lectins. **Y. Ebara***, Y. Nomura, M. Matsuda, M. Yamabe, D. Akamatsu

9:45 break

10:00 – 174. Synthetic receptors for carbohydrates. **A. Davis***

10:30 – 175. Analysis of ER glucosidase transferase by means of chemical synthesis. **Y. Ito**

11:00 – 176. Metabolic glycan labeling using liposomal unnatural sugars. **X. Chen**

11:30 – 177. Synthesis of designer polysaccharides as probes of glycan function. **T. Lowary**

Sheraton Waikiki
Kahuku

Lucifer/Luciferase Engineering (#410)

Organized by: M. Pirrung, M. Li,
M. Hiyama
Presiding: M. Pirrung

8:00 Coffee

8:30 – 178. Beyond D-luciferin: A bright future for bioluminescence. **S.C. Miller***

9:00 – 179. Imaging cell-cell contacts with engineered bioluminescent tools. **J. Prescher***

9:30 – 180. Reaction-based luciferin probes for in vivo metal and redox imaging. **C.J. Chang***

10:00 – 181. Structural variations enhancing the bioluminescence of luciferin. **M. Pirrung***, A. Dorsey, N. De Howitt, J. Liao

10:30 – 182. Mystery of firefly bioluminescence revealed?. **P. Naumov***, M. Siwa, L. Hintermann, P. Didier

11:00 – 183. Expand the scope of bioluminescence from firefly luciferase/luciferin system. **M. Li***

Hawaii Convention Center
Halls I, II, III

Chemical Biology of Protein-Lipid Modification (#421)

Organized by: M. Distefano, J. Ohkanda, Y. Chen

Poster Session

10:00 – 12:00

184. Glutathione adduct of methylmercury activates Nrf2 through covalent modification of Keap1 in SH-SY5Y cells. **Y. Kumagai**

185. Liver cell specific targeting by myristoylated preS1-conjugated nanogages for drug delivery. **M. Murata***, J. Piao, S. Narahara, T. Kawano, N. Hamano, M. Hashizume

Sheraton Waikiki
Honolulu

The RNA World: From Prebiotic Chemistry to the Emergence of Complexity (#449)

Organized by: N. Hud, P. Unrau, Y. Furukawa
Presiding: P.J. Unrau

8:00 – 186. Meteorite impacts and abiotic formation of RNA components. **Y. Furukawa***, H. Nakazawa, T. Sekine, T. Kobayashi, T. Kakegawa

8:30 – 187. Resolving paradoxes in the origin of life: The interface between mineralogy and organic chemistry. **S. Benner***, H. Kim, J. Kawai

9:00 – 188. Self-assembly approach to proto-RNA. **N. Hud***

9:30 15 min Break

9:45 – 189. Emergence of RNA. **R. Krishnamurthy***

10:15 – 190. Iron and the primordial biochemistry of nucleic acids. **L. Williams***

10:45 15 min Break

11:00 – 191. Ribozymes that catalyze tRNA aminoacylation. **N. Terasaka**, S. Ishida, H. Suga*

11:20 – 192. Spontaneous assembly of an organic-inorganic nucleic acid Z-DNA double helix structure. **L. Cronin***

11:40 – 193. Abiotic synthesis of nucleic acid bases from possible interstellar media by particles irradiation. **K. Kobayashi***, H. Tokimura, Y. Kebukawa, T. Kaneko, H. Fukuda, Y. Oguri, S. Yoshida

* Principle Author

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Wednesday Afternoon

Sheraton Waikiki
Ewa

Low-Energy Photoexcited States in Photosynthesis (#117)

Organized by: J. Reimers, E. Krausz, A. Freiberg, D. Bruce, A. Holzwarth, H. Hashimoto, D. Coker
Presiding: A. Freiberg

13:00 – 194. Different strategies to collect light in photosynthesis: A bottom up theoretical approach. **T. Renger**, A. Klinger, F. Steinecker, M. Schmidt am Busch, F. Mühl

13:30 – 195. Low energy forms of photosystem I in plants and green algae. **R. Croce***

14:00 – 196. Spectroscopic evidence for modulation of the carotenoid -bacterio-chlorophyll interactions in assembly of the core LH1-RC complex of photosynthetic bacteria. **A. Freiberg***, J. Linnanto, M. Rätsep

14:30 Afternoon tea

15:00 – 197. Chlorophyll c and the paradox of light-harvesting in chromophyte algae. **A.W. Larkum**

15:30 – 198. Structural basis for the unusual red-shift of the LH1 Qy transition of LH1-RC core complex from *Thermochromatium tepidum*. T. Kawakami, L. Yu, Z. Wang-Otomo*

16:00 – 199. Low energy excited states: Successes and challenges. **J. Reimers**

Royal Hawaiian
Regency III

Advances in Biological Solid-State NMR (#120)

Organized by: A. Naito, M. Auger, A. Ramamoorthy, F. Separovic, T. Fujiwara, Y. Kim
Presiding: A. Naito, F. Separovic

13:00 – 200. NMR approaches to view high-resolution interactions of Cytochrome P450 with its REDOX partners in a membrane environment. M. Zhang, K. Yamamoto, R. Huang, S. Im, L. Waskell, **A. Ramamoorthy***

13:25 – 201. Proton conduction mechanism in the cytoplasmic-containing influenza M2 protein and new solid-state NMR techniques for membrane protein structure determination. **M. Hong***, S. Liao, B. Kwon, J. Williams, T. Wang, P. White

13:50 – 202. NMR studies of lipid rafts. **N. Matsumori**, T. Yasuda, T. Yamaguchi, M. Murata

14:15 – 203. NMR studies of lipid-associated proteins in complex systems. **V. Booth**

14:40 – 204. Solid-state NMR studies for chromophore-protein interaction changes in pharaonis phorborhodopsin.

I. Kawamura*, R. Nishikawa, S. Nakatani, T. Okitsu, A. Wada, N. Kamo, A. Naito

14:55 Break

15:10 – 205. Solid-state NMR structural studies of antimicrobial peptides with enhanced activities. **Y. Kim***, J. Kim, J. Jeong

15:35 – 206. Localisation of the antimicrobial peptide maculatin 1.1 in anionic bicelles using solid-state NMR. **M. Sani***, F. Separovic

16:00 – 207. Solid-state NMR studies of crystalline state DMPC and a synthetic mimic of GPI-anchored protein in membranes. **K. Nomura***

16:25 – 208. Solid-state NMR of membrane proteins: From 6 kDa transmembrane domains to 2MDa membrane protein complexes. **G. Veglia***

Sheraton Waikiki
Kauai

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

Organized by: Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang
Presiding: C. Arrowsmith

13:00 – 209. Chemical probes for chromatin regulators. **C. Arrowsmith***

13:30 – 210. Gripping histone acetylation mark with YEATS domain. **H. Li***, Y. Li, H. Wen, Y. Xi, W. Li, X. Shi

13:55 – 211. Binding mechanisms and specificities of epigenetic readers. J. Gatchalian, M. Ali, F. Andrews, B. Klein, Q. Tong, R. Rosas Ospina, T. Kutateladze*

14:20 – 212. Functional interplay between epigenetic DNA modifications and RNA polymerase II transcriptional machinery. **D. Wang***

14:45 Break

14:55 – 213. From epigenetic mechanism to targeted therapy. **M. Zhou***

15:20 – 214. Protein methyltransferases: Structure and inhibition. **M. Schapira***

15:45 – 215. Aromatic amino acids: Privileged side-chains for bromodomain ligand discovery. **W.C. Pomerantz***, N. Mishra, A. Urick, S.W. Ember, E. Schonbrunn

16:10 – 216. Oligomerization of protein arginine methyltransferase 8 and a novel regulatory site for substrate specificity. **M. Ho***

16:35 – 217. Identification and crystallographic analysis of a small molecule selective SIRT2 inhibitor. **A. Ito**, N. Kudo, A. Nakata, S. Maeda, M. Yoshida*

Sheraton Waikiki
Maui

Strategies for Coupling and Decoupling Diverse Molecular Units in the Glycosciences (#201)

Organized by: Z. Witczak, M. Brimble, Y. Miura, R. Bielski
Presiding: M.A. Brimble, Y. Miura

13:00 – 218. Levoglucosanone, a not so new but now abundant and highly versatile chiron. **M.G. Banwell***

13:30 – 219. Large-scale production of levoglucosanone and dihydrolevoglucosanone from cellulosic wastes and residues. **C. Gunawan***, J. Clark, A. Constantinou, G.R. Court, M. De Bruyn, T. Duncan, T.J. Farmer, A.J. Hunt, S.G. Lawrence, R. McElroy, L. Moity, W.D. Raverty, J. Sherwood

14:00 – 220. Sequential thiols recognition in coupling of functionalized carbohydrates. **Z. Witczak***, R. Bielski

14:30 – 221. Enzymatic strategies to glycan synthesis. **S.L. Flitsch**

15:05 Break

15:15 – 222. Application of the inverse-electron-demand Diels-Alder reaction for the visualization of cellular carbohydrates. **V. Wittmann***

15:50 – 223. Palladium-triggered activation of cytotoxic glycosides: An unorthodox use of the biorthogonal concept. **A. Unciti-Broceta***

16:25 – 224. Sacrificial units in coupling and decoupling (CAD) of diverse molecules. **R. Bielski*, Z. Witczak**

16:55 Concluding Remarks

Royal Hawaiian
Regency I

Enzyme Engineering and Biocatalysis Applications (#222)

Organized by: J. Pelletier, S. Lutz, B. Kim, R. Kazlauskas, N. Itoh
Presiding: J. Pelletier

13:00 – 225. Enzyme engineering as an enabling tool for synthetic biology/chemistry. **H. Zhao**

13:20 – 226. Continuous evolution of proteins with novel therapeutic potential. **D.R. Liu**

14:00 – 227. Site-directed mutagenesis of the human ITPAse substrate specificity pocket. **N.E. Burgis***

14:20 – 228. Metalloenzyme design using genetic code expansion. **J. Wang***

14:40 COFFEE BREAK

14:50 – 229. Protein engineering using “small, but smart” mutant libraries. **U.T. Bornscheuer***

15:10 – 230. Engineering an enzyme complex that exhibits substrate channeling. **S. Seah***

15:50 – 231. Novel enzymes and synthetic pathways for sustainable chemicals. **D. Grabs**, E. Althoff, Y. Ban, M. Galzicki, R. Azzopardi, A. Zanghellini

16:10 – 232. Substrate-selecting mechanism of alcohol and phenol sulfotransferases. **Y. Yang***

Sheraton Waikiki
Molokai

Physiology and Metabolism of Extremophiles (#249)

Organized by: H. Atomi, J. Reeve, M. Ito, S. Kang
Presiding: H. Atomi

13:00 – 233. Formation of P-N, P-S and P-O bonds by a single archaeal enzyme. R.G. Brinson, J. Shin, Y. Simori-Manso, S. Li, J.P. Marino, Z. Kelman*

13:25 – 234. Structure and functions of the Thermococcal-specific exonuclease. **S. Ishino***, K. Miyazono, T. Yamagami, T. Hamasuna, T. Shirai, H. Tomita, T. Kanai, H. Atomi, M. Tanokura, Y. Ishino

13:50 – 235. Characterization of an archaeal hyperthermophilic cellulase expressed in *plantae*. Glycosylation, activity, and substrate specificity. **P. Bubner**, H. Szemenyi, S. Tang, D. Clark, C. Somerville

14:15 – 236. Geographical characteristic of piezophiles. **M. Kusube**, M. Inoue, K. Tanikawa, D.H. Bartlett

14:40 Break

14:50 – 237. Histones, chromatin structure, and genome expression in hyperthermophilic Archaea. **J. Reeve***, K. Sandman, D. Jaeger, Y. Fondufe-Mittendorf, T. Santangelo, S. Bhattacharyya, P. Dyer, K. Luger

15:15 – 238. Cold-stress response and adaptation in hyperthermophilic archaea. **S. Fujiwara***

15:40 – 239. Enhancing effect of thermostable archaeal helicases on the PCR specificity. **A. Fujiwara**, K. Yasukawa, S. Fujiwara

16:00 – 240. Physiological and transcriptional response of *Thermus scotoductus* SA-01 to dielectric heating. **J.C. Biffinger***, A. Cockrell, K.D. Cusick, J. Dale, J. Baldwin, S. Tsai, L.A. Fitzgerald, D.E. Barlow, C. Soto, S. Strycharz-Claven, B. Lin, A. Malanoski, J. Cramer, R. Morris, B. Little

16:25 – 241. Studies on the adaptive changes of a hyperthermophilic archaeon *Thermococcus onnurineus* NA1 under long-term selection on carbon monoxide. **S. Kang***, S. Lee, M. Kim, J. Lee, J. Lee, H. Lee

16:50 Closing Remarks

Sheraton Waikiki
Lanai

Carbohydrate Recognition in Health and Disease (#342)

Organized by: G. Boons, Y. Ito, A. Demchenko, D. Vocadlo

13:00 – 242. Glycosaminoglycan recognition and signaling in the brain. **L. Hsieh-Wilson***

13:30 – 243. Novel glycosidase inhibition motifs found in amylase inhibitors.

S.G. Withers*, G.D. Brayer, R. Andersen, L. Williams, X. Zhang, C. Tysoe, C. John, R. Keyzers, J. McNeill, V. Yuen, D. Williams, S. Caner, N. Nguyen

14:00 – 244. Newborn screening for lysosomal storage diseases: Clinical carbohydrate enzymology from research to product. **M.H. Gelb**

14:30 – 245. Understanding the roles of complex glycolipids in innate immunity through chemical synthesis.

M. Richardson, P. van der Peet, S. Shah, **S.J. Williams***

14:45 break

15:00 – 246. Target-selective photodegradation of oligosaccharides in health and disease. **K. Toshima***

15:30 – 247. Glycopeptide vaccines for cancer immunotherapy. **Y. Li**

16:00 – 248. Druggability of lectins, using the example of a bacterial adhesin. **B. Ernst***, P. Frei, J. Bezencon, D. Eris, R. Preston

16:30 – 249. Analysis of mucin-type O-glycans in tumor cells by saccharide primer method. **R. Sakura**, Y. Takahashi, T. Sato*

16:45 – 250. Analyses of glycans expressed in human hepatoma cells sensitive to hepatitis C virus. **H. Yamaguchi***, T. Suzuki, T. Sato

Sheraton Waikiki
Kahuku

Luciferin/Luciferase Engineering (#410)

Organized by: M. Pirrung, M. Li, M. Hiyama
Presiding: M. Li

13:00 – 251. Theoretical study for photoluminescence of firefly-bioluminescence-related molecules. **M. Hiyama***, Y. Noguchi, T. Mochizuki, K. Yamada, H. Akiyama, N. Koga

13:30 – 252. Bioluminescence multicolor imaging and assay using secreted and non-secreted luciferases. **Y. Ohmiya**

14:00 – 253. Characterization of the luciferase active site for the color modulation mechanism in firefly bioluminescence. **T. Hirano**

14:30 – 254. Hinge region engineering of firefly luciferases for robust protein-protein interaction assay *FilmPIA*. **H. Ueda***, H. Yamaji, Y. Ohmuro-Matsuyama

15:00 – 255. Luminous reaction analysis of firefly luciferin analogs. **M. Kiyama***, R. Obata, T. Hirano, S. Maki

15:30 – 256. Study on the color modulation mechanism of firefly bioluminescence with an amine substituent effect of luciferin and oxyluciferin. **M. Kakiuchi**, M. Yamaji, S. Maki, T. Hirano*

Sheraton Waikiki
Honolulu

The RNA World: From Prebiotic Chemistry to the Emergence of Complexity (#449)

Organized by: N. Hud, P. Unrau, Y. Furukawa
Presiding: Y. Furukawa

13:00 – 257. Role of chance in the evolution of early life. **I. Chen**

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- 13:30 – 258.** Evolving increasing complexity in the RNA world. **P. Higgs***
- 14:00 – 259.** RNA membrane vesicle: Micro compartment made by designed RNA molecules. **S.M. Nomura**, H. SAITO, M. Takinoue, K. Fujiwara, H. OHNO
- 14:30** 15 min Break
- 14:45 – 260.** Ribozymes that utilize heme and thiamin as cofactors. **D. Sen***, P. Cernak, N. Shumayrikh, J. Grigg
- 15:15 – 261.** Von Neumann, and Turing with RNA: The challenges inherent in building and understanding self-replicating RNA machines. **P.J. Unrau**
- 15:45** 15 min Break
- 16:00 – 262.** Experimental RNA evolution in droplets: How cellularity contributes the early RNA world evolution. **S. Matsumura**, F. Coldren, A. Kun, P. Nghe, F. Jossinet, E. Szathmary, A. Griffiths*, M. Ryckelynck
- 16:20 – 263.** In vitro selection of peptides with enhancing effect for the RNA polymerase ribozyme. **S. Kumachi**, N. Nemoto

Wednesday Evening

Sheraton Waikiki
Honolulu

New Platforms for Natural Products Discovery (#18)

Organized by: G. Carter, R. Andersen, B. Copp, S. Matsunaga
Presiding: G. Carter

- 19:00 – 264.** Discovery of novel chlorinated acyl amides from a marine cyanobacterium using integrated genome mining and MS-based molecular networks. **W. Gerwick***, K. Kleigrewe, J. Almaliti, I. Tian, R. Kinnel, A. Korobeynikov, E. Monroe, B. Duggan, V. Di Marzo, D. Sherman, P. Dorrestein, L. Gerwick
- 19:40 – 265.** Biologically active natural products: Discovery, SAR, and interactions with protein targets. **R. Andersen***
- 20:20 – 266.** Search for marine natural products with anticancer associated activity. **S. Matsunaga***

Sheraton Waikiki
Waialua

Advances in Biological Solid-State NMR (#120)

Organized by: A. Naito, M. Auger, A. Ramamoorthy, F. Separovic, T. Fujiwara, Y. Kim
Presiding: M. Auger

- 19:00 – 267.** Solid-state NMR relaxometry and structural deformation in biomembrane function. **M.F. Brown***, X. Xu, J.J. Kinnun, A. Leftin, S. Lee, K.J. Mallikarjuniah, T.R. Molugu, A.V. Strutis
- 19:25 – 268.** NMR relaxation in solid proteins and peptides: Insights into protein dynamics and structure. **K.W. Zilm**
- 19:50 – 269.** Influenza virus fusion peptide-induced membrane acyl chain hairpins detected by paramagnetic enhancement of ²H relaxation. **S. Liang**, D. Weliky
- 20:05 – 270.** Hierarchy of picosecond to microsecond anisotropic protein motions. **J.M. Lamley, R. Stevens, J. Lewandowski***
- 20:20 – 271.** Intrinsic disorder and conformational heterogeneity: Surprising complexities from membrane proteins. **T. Cross***, N. Das, Y. Miao, C. Escobar, V. Ekanayake, A. Wright, J. Paulino, J. Dai, M. Rajagopalan, H. Zhao
- 20:45** Closing Remarks

Hawaii Convention Center
Halls I, II, III

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

Organized by: Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang

Poster Session

19:00 – 21:00

- 272.** Regulation of histone modifications in telomere by G-quadruplex telomere DNA and TERRA binding protein. **T. Oyoshi**
- 273.** Acetylation of the nucleoprotein of influenza A virus by GCN5 and PCAF. D. Hatakeyama, M. Shioji, R. Yoh, N. Ohmi, S. Takenaka, S. Yamayoshi, Y. Arakaki, T. Komatsu, A. Masuda, M. Nakano, T. Noda, Y. Kawaoka, T. Kuzuhara*
- 274.** Identification of lysine demethylase 5A inhibitors and their effect on cancer cells. **Y. Itoh**, H. Sawada, M. Suzuki, T. Mizukami, T. Suzuki
- 275.** DNA methylation pattern analysis of common plant virus promoter used to develop genetically modified crops. **K. Nakamura***, T. Ishigaki, K. Hanada, S. Akimoto, K. Kondo, T. NISHIMAKI-MOGAMI
- 276.** Developing novel photoaffinity probes to identify 'readers' of histone modifications. **X. Li**, T. yang, X.D. Li*
- 277.** Effects of epigenetic modifications on the binding of histone tail peptides with DNA strands. **K. Murata**, S. Higashida, S. Pramanik, N. Sugimoto, D. Miyoshi*
- 278.** Discovery of dual-functional anticancer drugs using LSD1 inhibition as a trigger. **Y. Ota**, Y. Itoh, T. Suzuki*
- 279.** Isoform-selective protein arginine methyltransferase inhibitors. **K. Qian**, Y. Zheng*
- 280.** Synthesis strategy of linker histone H1 for chromatin research. **R. Sakamoto**, G. Hayashi, A. Okamoto*
- 281.** Molecular basis for N-terminal tri-methylation of CENP-A by NMT1. **R. Wu***
- 282.** Identification of lysine glutarylation as a new type of histone modification. **X. Bao***, Y. Xiong, Y.E. Fung, X.D. Li
- 283.** Search for active components of Japanese "miso" affecting histone modification and neural differentiation. **S. OTSUKA**, K. Sugie, K. MACHIDA, D. Arai, Y. Hayashi-Takanaka, H. Kimura, Y. Nakao
- 284.** Isolation and structure elucidation of an active compound affecting histone modification from the marine sponge. **K. MACHIDA***, N. Ishibashi, R. Kataoka, D. Arai, Y. Hayashi-Takanaka, H. Kimura, N. Fusetani, Y. Nakao
- 285.** Application for live-cell imaging with chemically synthesized histone H2A. **T. Sueoka**, G. Hayashi, A. Okamoto*
- 286.** Toward SIRT7 inhibitors: From screening of known SIRT1-3 modulators to de novo-design. **P. Mellini**, Y. Itoh, T. Kakiizawa, M. Lahtela-Kakkonen, E. Jarho, S. Valente, D. Rotili, A. Mai, T. Suzuki*
- 287.** Development of a genetically encoded FRET indicator for intra-nucleosomal histone H3 lysine 9 tri-methylation and live-cell imaging. **K. Sasaki***, M. Suzuki, A. Ito, K. Shin-ya, M. Sodeoka, Y. Nakao, M. Yoshida
- 288.** Integrative chemical biology approaches for examining "erasers" for fatty acid acylation of lysine residues in proteins. **Z. Liu***, T. yang, X. Li, X.D. Li
- 289.** Interaction between arginine methylation and serine phosphorylation in histone H3. **M. Mendoza**
- 290.** Probing lysine acetyltransferase substrates with clickable acetyl-CoA analogs and engineered enzymes. **Z. Han***, Y. Zheng
- 291.** Construction and screening of a focused library for histone demethylase inhibitors. **B. Li**, Y. Ota, Z. Hui, Y. Itoh, T. Suzuki
- 292.** Investigation of DNA demethylation by Tet protein. **S. Kizaki**, Y. Suzuki, A. Chandran, Y. Han, M. Endo, Y. Harada, H. Sugiyama*
- 293.** Selective chemical probes of protein arginine methyltransferases. **H. Hu**, Y. Zheng*
- 294.** New biochemical assays for the histone acetyltransferases. **L. Ngo**, Y. Zheng*
- 295.** Crystal structure of PARG provides insight into molecular mechanism of poly ADP-ribose turnover for epigenetic regulation. **C. Hsu***, C. Cho, M. Lin, Y. Chang
- 296.** Identification of histone deacetylase 1/2-selective inhibitors using click chemistry-based combinatorial fragment assembly. **Z. Hui**, P. Zhan, T. Tojo, Y. Itoh, T. Suzuki
- 297.** 2.2 Å crystal structure of Bre1-RING finger domain. **S. Zhao***, X. Su, H. Li
- 298.** Developing chemical tools to study histone acetyltransferases. **X. Li***, X. Bao, X.D. Li
- Hawaii Convention Center
Halls I, II, III
- Physiology and Metabolism of Extremophiles (#249)**
- Organized by: H. Atomi, J. Reeve, M. Ito, S. Kang
- Poster Session**
- 19:00 – 21:00**
- 299.** Protective effects of tartary buckwheat flavonoids against high TMAO diet-induced vascular dysfunction and liver injury in mice. **X. Yang***, Y. Hu*
- 300.** Lipid characteristics of a steep clam, *Mesolinga solidifesta*: Comparison with those of two coastal clams. **h. saito***
- 301.** Studies on the physiological function and biochemical properties of the *frhAGB*-encoding hydrogenase from a non-methanogenic hyperthermophilic archaeon. **H. Lee**, J. Jeon, J. Lim, J. Lee, S. Kang*
- 302.** Effects of salt on the structure, stability, and function of a halophilic dihydrofolate reductase. **Y. Miyashita**, E. Ohmae*, K. Nakasone, K. Katayanagi
- 303.** Co-cultivation with *Methyllobacterium* sp. ME121 and *Kaistia* sp. 32K increased swimming velocity of ME121. **Y. Wakabayashi***, T. Shimizu, A. Nakamura, M. Ito
- 304.** Structural analysis of PilQ from *Thermus thermophilus*. **T. Maruyama**, A. Sasaki, M. Tamakoshi, A. Koike-Takeshita*
- 305.** Functional analysis of Φ TMA-encoded GroES-like protein. **K. Kondo**, M. Tamakoshi, A. Koike-Takeshita*
- 306.** Characteristics of microbial water gas shift reaction by carboxydrotrophic archaeon *Thermococcus onnurineus* NA1 with various carbon monoxide concentrations. **J. Na**, H. Jeong, D. Jin, T. Kim*, S. Chung, S. Kang, T. Jung*
- 307.** *gaa* and *glgX* genes are responsible for the glycogen degradation in thermoacidophilic archaeon *Sulfolobus acidocaldarius*. **J. Cha***, J. Park, K. Choi, Y. Seo, Y. Jung
- 308.** Computational prediction of novel nucleases involved in tRNA maturation in hyperthermophilic prokaryotes. **D. Matelska**, K. Ginalski*
- 309.** Medium optimization for enhancement of formate-driven biydrogen production by the hyperthermophilic archaeon, *Thermococcus onnurineus* NA1. **T. Kim**, S. Lee, H. Lee, J. Lee, J. Na*, S. Kang*
- 310.** Elucidation of the reduced motility mechanism of alkaline *Bacillus* at low pH. **Y. Takahashi**, Y. Noguchi, M. Ito
- Hawaii Convention Center
Halls I, II, III
- Frontiers of Iron Chemistry in Biology (#268)**
- Organized by: K. Ishimori, S. Sliger, G. Mauk
- Poster Session**
- 19:00 – 21:00**
- 311.** Stopped-flow kinetic analysis of human duodenal cytochrome *b*₅₆₁. **H. Takeda***, H. Togashi, T. Kimura, G. Mauk, H. Sugimoto, Y. Shiro
- 312.** Development of a time-resolved visible/IR absorption spectrometer with a novel microfluidic device and its application to catalytic reaction of NO reductase. **T. Kimura**, S. Ishii, T. Toshia, Y. Shiro*, M. Kubo*
- 313.** Cytoplasmic heme-binding protein (HutX) from the heme utilization system of *Vibrio cholerae* is an intracellular heme-trafficking protein for the heme degrading enzyme, HutZ. **Y. Sekine***, K. Ishimori, T. Uchida
- 314.** Identification of functionally critical residues for NO reduction of nitric oxide reductase from *Pseudomonas aeruginosa* by *in vivo* and *in vitro* mutagenesis analyses. R. Yamagawa, H. Sawai, T. Toshia, H. Nakamura, H. Arai, Y. Shiro*
- 315.** Unique heme degradation catalyzed by IscG-type enzymes from *Staphylococcus aureus*. **T. Matsui***, S. Nambu, Y. Ono, M. Tsunoto, M. Ikeda-Saito*
- 316.** Heme degradation by the heme oxygenases from different biological species: Discrimination of their heme-cleavage kinetics. **C.T. MIGITA***, N. Miyake, T. Matsui, S. YANAGISAWA, T. OGURA, M. Ikeda-Saito
- 317.** Microbial biosynthesis of terminal alkenes and alkynes. **X. Zhu**, Z. Rui, W. Zhang
- 318.** Enhanced MRI relaxivity induced by novel 1D Fe₃O₄ building blocks. **J. Beltran-Huarac***, D. Diaz-Diestra, J. Vilmenay, B.R. Weiner, G. Morell
- 319.** Expression of an oxygen-stable group III alcohol dehydrogenase from the hyperthermophilic archaeon *Pyrococcus horikoshii* OT3. **C. Sugimoto**, K. Takeda, M. Yohda, N. NAKAMURA*, H. Ohno
- 320.** Improvement of expression and purification systems for thermophilic cytochrome P450. **N. Tsuruoka**, S. Hayakawa, K. Takeda, M. Yohda, N. NAKAMURA*, H. Ohno
- 321.** Zinc(II) facilitates interaction between the multicopper ferroxidase ceruloplasmin and the iron transporter transferrin resulting in safe transfer Fe(III) from the former enzyme to the latter protein. **T. Yamamura***, T. Sakajiri
- Hawaii Convention Center
Halls I, II, III
- Luciferin/Luciferase Engineering (#410)**
- Organized by: M. Pirrung, M. Li, M. Hiyama
- Poster Session**
- 19:00 – 21:00**
- 322.** Highly selective bioluminescent probes for fluoride detection and the application in bioimaging. **B. Ke**
- 323.** Study of specific interactions of oxyluciferin with catalytic center of firefly luciferase by computational analysis of titration curves of its some amino acid residues. **H. Sakai***, S. Takamatsu, N. Wada
- 324.** Development of non-CRET based orange chemiluminescent imidazo[1,2-*a*]pyrazin-3(7H)-ones. **R. Saito***, T. Hirano, S. Maki, H. Niwa
- 325.** Development of red-shifted luciferase mutants derived from Brazilian click beetle *Pyrearinus terminilluminans*. **T. Nishiguchi**, T. Yamada, Y. Nasu, H. Yoshimura, T. Ozawa*
- 326.** Role of luciferase in myrFMN formation. **E. Brodin***, C. Tabib, T. Bergner, J. Ivkovic, R. Breinbauer, P. Macheroux

* Principle Author

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- 327.** Imaging system for monitoring of intracellular acidification in living tissues by photocontrollable luciferase. **M. Hattori**, T. Ozawa*
- 328.** Creation of artificial luciferases and their application to bioassays. **S. Kim**

Hawaii Convention Center
Halls I, II, III

The RNA World: From Prebiotic Chemistry to the Emergence of Complexity (#449)

- Organized by:* N. Hud, P. Unrau,
Y. Furukawa
- Poster Session**
19:00 – 21:00
- 329.** Effect of clay minerals on the evolution of RNA function. **J.D. Stephenson***, P.S. Fliss, M. Popovic, M.A. Ditzler
- 330.** Prebiotic flow synthesis of bioactive nucleoside precursors. **A. Evans**, J. Kading, J. Feng
- 331.** UV photochemistry of prebiotic nucleobases. **M.S. de Vries**
- 332.** Non-enzymatic ribonucleotide reduction in the prebiotic context. **D.M. Smith***
- 333.** Difficulty of spontaneous formation and replication of oligonucleotides containing 4 kinds of nucleotide residues using the monomeric activated nucleotides. **K. Kawamura***
- 334.** Emergence of RNA self-replication cycle through RNA template-directed RNA polymerization by DNA dependent RNA polymerase. **Y. Kakimoto***, A. Fujinuma, Y. Kikuchi, S. UMEKAGE*
- 335.** Overcoming strand inhibition using viscous environments. **C. He***, I. Gallego, B. Laughlin, N. Hud, M. Grover

Thursday Morning

Royal Hawaiian
Regency II

New Platforms for Natural Products Discovery (#18)

- Organized by:* G. Carter, R. Andersen, B. Copp, S. Matsunaga
Presiding: S. Matsunaga
- 8:00 – 336.** Sterol-targeting antibiotics and the balance of membrane trafficking. **S. Nishimura**, H. Kakeya
- 8:35 – 337.** Natural product library design for fragment-based screening using bioaffinity mass spectrometry. **R.J. Quinn***
- 9:10 – 338.** Mass imaging as a tool to study the unique natural products of plant and invertebrate microbiomes. **M.T. Hamann**
- 9:45 Break**
- 10:15 – 339.** Natural products-based screening study on disease and development pathways. **M. Ishibashi***
- 10:50 – 340.** Development of in vitro and in vivo fluorescence imaging systems for chemical screening. **Y. Miwa***, Y. Nakao, J.K. Tanaka, S. Takahashi
- 11:25 – 341.** Adhesion of alive mycolic acid-containing bacteria during the induction of secondary metabolism in *Streptomyces*. **S. Asamizu***, T. Ozaki, K. Satoh, K. Teramoto, H. Onaka*

Sheraton Waikiki
Ewa

Characterization and Applications of Food Enzymes (#59)

- Organized by:* F. Chen, F. Chen, H. Ni, Y. Lee
Presiding: F. Chen, H. Ni, D. Wong, J. Wu
- 8:00 Introductory Remarks**
- 8:05 – 342.** Preparation and application of *Thermobifida fusca* cutinase. **J. Wu**, L. Su, X. Duan
- 8:35 – 343.** From metagenomic gene discovery to enzymatic breakdown of crosslinks in agricultural fibers for functional products. **D. Wong***, V. Chan, M. Murakami
- 8:55 – 344.** Optimizing heterologous protein production in food-grade lactic acid bacteria with fusion partners. P. Lim, **F. Wong**, D. Ow*

- 9:15 – 345.** Characterization of β -aspartyl-transferase from *Deftia acidvorans*. **R. Naohara***, A.A. Pribanto, Y. Nonomura, K. Takagi, M. Umekawa, M. Wakayama
- 9:35 – 346.** Microparticle-enhanced production of ferulic acid esterases by submerged cultivation of *Aspergillus niger* ZJUQH and its application for production of ferulic acid from wheat bran. **Q. Chen**
- 9:55 Session Breaks**
- 10:05 – 347.** First characterization of an acidic D-psicose 3-epimerase from *Dorea* sp. CAG317. **W. Mu**
- 10:25 – 348.** Effect of glycosylationon catalytic characteristics and stability of tannase from *Aspergillus niger* JXF02. **G. Fu***, C. Liu, S. Luo, J. Wu, P. Zhou, L. Gao, S. Wang
- 10:45 – 349.** Purification and characterization of an α -L-rhamnosidase from the solid-state fermentation product of *Aspergillus tubingensis*. **H. Ni***, S. Wang, F. Chen, H. Cai, A. Xiao, G. Su
- 11:05 – 350.** Characterization and gene cloning of proteases from *Lentinula edodes*. **Y. Fukuta**, T. Iwanaga, T. Terashita, N. Shirasaka
- 11:25 – 351.** Gene cloning, expression, and biochemical characterization of two novel cold-active lipases from *Rhizomucro endophyticus*. **S. Yang***

Hawaii Convention Center
Halls I, II, III

Advances in Biological Solid-State NMR (#120)

- Organized by:* A. Naito, M. Auger, A. Ramamoorthy, F. Separovic, T. Fujiwara, Y. Kim
Presiding: T. Fujiwara, Y. KIM

Poster Session

10:00 – 12:00

- 352.** Membrane interaction and calcium myristoyl switch of recoverin: A ^2H and ^{31}P solid-state NMR study. **K. Potvin-Fournier***, G. Valois-Paillard, C. Salesse, M. Auger
- 353.** Interaction of Bombinin H4 containing a D-amino acid residue with lipid membranes as studied by solid-state NMR and MD simulations. **Y. Kitahashi***, N. Javkhlanjuts, S. Kaneda, N. Altannavach, K. Ueda, A. Naito, I. Kawamura
- 354.** Hydrogen bond alterations of Tyr174 and Tyr199 of phorbophilopsin in the lipid environment as studied by solid-state ^{13}C MAS NMR. **R. Nishikawa***, I. Kawamura*, T. Okitsu, A. Wada, Y. Sudo, N. Kamo, A. Naito
- 355.** Structural changes in the photo-reaction pathways of retinal in bacteriorhodopsin studied by in-situ photo-irradiation solid-state NMR. **A. Shigeta***, K. Oshima, R. Miyasa, M. Horigome, I. Kawamura, T. Okitsu, A. Wada, S. Tuji, A. Naito
- 356.** Structural diversity of amyloid fibril and its intermediate in human calcitonin as studied by solid-state NMR and MD simulation. **S. Toyoda***, L. Ganchimeg, N. Javkhlanjuts, H. Itoh-Watanabe, I. Kawamura, K. Ueda, A. Naito
- 357.** Photo reaction pathways of sensory rhodopsin I as revealed by in-situ photo-irradiation solid-state NMR. **Y. Makino***, H. Yomoda*, Y. Tomonaga, T. Hidaka, I. Kawamura, T. Okitsu, A. Wada, Y. Sudo, A. Naito
- 358.** H^+ -translocation of thermophilic F_0F_1 -ATP synthase c-subunit rings investigated using solid-state NMR. **S. Kang**, **Y. Todokoro**, I. Yumen, B. Shen, I. Iwasaki, T. Suzuki, A. Miyagi, M. Yoshida, T. Fujiwara, H. Akutsu

Sheraton Waikiki
Kauai

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

- Organized by:* Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang
Presiding: Y. Nakao

8:00 – 359. New tools for studying chromatin biochemistry. **T. Muir**

- 8:30 – 360.** Use structurally defined nucleosomes to profile epigenetic targets of histone lysine deacetylases and demethylases. **W. Liu**

8:55 – 361. Proteomic approaches for epiproteome analysis. **A. Tackett**

- 9:20 – 362.** Modified histone proteins in the test tube and the cell. **J.J. Ottesen***

9:45 Break

- 9:55 – 363.** Understanding aberrant methylation patterns on histones in b-cell cancers. **N.L. Kelleher***

10:25 – 364. New approach to study histone modification changes controlling biological phenomena by small molecules. **Y. Nakao***, D. Arai, Y. Kina, R. Kataoka, Y. Hayashi-Takanaka, H. Kimura

- 10:50 – 365.** Chemical strategies to investigate histone sumoylation. **C. Chatterjee***

11:15 – 366. Allele-specific chemical genetics for the functional elucidation of chromatin modifiers. **K. Islam***

- 11:40 – 367.** Bio-inspired synthetic DNA-based epigenetic switches for pharmaceutical gene modulation. **G. NAMASIVAYAM**, S. Sato, J. Taniguchi, J. Syed Jabarulla, T. Bando, G. Kashiwazaki, H. Sugiyama

Royal Hawaiian
Regency III

Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

- Organized by:* M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada
Presiding: I. Shimada

8:00 Opening Remarks

- 8:15 – 368.** Studies of integral membrane proteins in nanodiscs. **G. Wagner***

8:45 – 369. How does cholesterol promote amyloidogenesis and Alzheimer's disease? **C. Sanders***

- 9:15 – 370.** Structure and interaction of F_0c -ring and lipid membranes for efficient energy transfer. **H. Akutsu**

9:45 – 371. Membrane interaction and conformational equilibrium of nanodisc-tethered KRAS and its oncogenic mutants. **M. Ikura***, M. Mazhab-Jafari, Z. Fang, M.J. Smith, C.B. Marshall

10:15 BREAK

- 10:30 – 372.** Functional analyses of target proteins for drug development by NMR. **I. Shimada***

11:00 – 373. How membranes determine function of lipoproteins, enzymes, and trafficking systems. **M. Overduin**, M. Lenoir, T. Knowles, I. Henderson, S. van Doren, I. Kufareva, R. Abagyan

- 11:15 – 374.** NMR-based drug design targeting membrane-bound proteins. **T. Haselhorst**

11:30 – 375. Molecular basis of voltage-gated ion channel inhibition by venom peptides. C.H. Lau, Y. Chin, J.K. Clint, G.F. King, **M. Mobli**

Sheraton Waikiki
Maui

Strategies for Coupling and Decoupling Diverse Molecular Units in the Glycosciences (#201)

- Organized by:* Z. Witczak, M. Brimble, Y. Miura, R. Bielski
Presiding: R. Bielski, M.A. Brimble

8:00 – 376. Syntheses and functions of glycosaminoglycan mimic polymers. **Y. Miura**, H. Seto, Y. Hoshino

- 8:30 – 377.** Glycoconjugate-based inhibitors of essential enzymes in *Mycobacterium tuberculosis*. S.K. Veleti, J.J. Lindenberger, S. Thanna, D.R. Ronning, **S. Suchek**

9:00 – 378. "Sugaring Tag" library. **T. Kitsunzuka**, K. Haneda, Y. Koda, T. Inazu

- 9:30 – 379.** Pyranoside-into-furanoside rearrangement: New reaction in carbohydrate chemistry and its application in oligosaccharide synthesis. V.B. Krylov, D.A. Argunov, A.G. Gerbst, **N.E. Nifantiev***

10:00 Break

- 10:10 – 380.** Synthesis and conformations of septanosides. **N. Jayaraman***, D. Supriya, N. Vijaya Ganesh

10:45 – 381. Sugar-based multicomponent coupling reactions for "Click" conjugation. **P.R. Andreana***

- 11:20 – 382.** New methods for the direct synthesis of glycoconjugates from reducing sugars in water. **A.J. Fairbanks***

11:55 Closing Remarks

Royal Hawaiian
Regency I

Enzyme Engineering and Biocatalysis Applications (#222)

- Organized by:* J. Pelletier, S. Lutz, B. Kim, R. Kazlauskas, N. Itoh
Presiding: N. Itoh

8:00 – 383. Controlled burning: Toward the rational redesign of O_2 and nonheme Fe(II) enzymes. **J. Niederhauser**, G. Straganz

- 8:20 – 384.** Enzymatic route toward the prenylation of linear and macrocyclic peptides. **S. Nair***, Y. Hao, E. Pierce, V. Agarwal, E.W. Schmidt

8:40 – 385. Innovation by evolution: Expanding the enzyme universe. **F.H. Arnold***

- 9:20 – 386.** Aldolase-catalyzed chemo-enzymatic syntheses of fine chemicals. **M. Sugiyama**

9:40 COFFEE BREAK

- 9:50 – 387.** Novel metabolic pathway of 3,6-anhydro-L-galactose for the red algae biorefinery. E. Yun, S. Lee, J. Yoon, I. Choi, **K. Kim***

10:10 – 388. Harnessing the promiscuity of natural product biosynthesis: A platform for engineering biosynthetic pathways with new specificities. **G.J. Williams***

- 10:30 – 389.** Enzymes from microbial, plant, and animal aldoxime-nitrile pathways and their applications. **Y. Asano**

11:10 – 390. Establishing high-level intracellular propionyl-CoA pool for biosynthesis of non-native chemicals in *Escherichia coli*. K. Srirangan, M. Moo-Young, **C. Chou**

Sheraton Waikiki
Lanai

Carbohydrate Recognition in Health and Disease (#342)

- Organized by:* G. Boons, Y. Ito, A. Demchenko, D. Vocadlo

8:00 – 391. Bioconjugates vaccines for the prevention of bacterial infections. **M.T. Kowarik**

*** Principle Author**

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8:30 – 392. Design, pre-clinical, and human clinical studies of the glycomimetic antagonists Rivipansel and GMI-1271 that target the selectins. **J. Magnani***

9:00 – 393. Synthesis of a 24-member library of heparin/heparan sulfate oligosaccharides for use in glycomics applications. **A.S. Campbell***, R. Laura, T. George, O. Plante

9:30 – 394. Glycophosphonate strategy for control of protein glycosylation: Discovery of fucosolphosphonate inhibitors of protein fucosylation in CHO cells. **J.G. Allen***

9:45 break

10:00 – 395. Us vs. them: Exploiting microbial cell surface glycosylation. **L.L. Kiesling**

10:30 – 396. Chemical synthesis of correctly folded and misfolded glycoproteins for understanding of glycoprotein quality control system. **Y. Kajihara***

11:00 – 397. Functional glycomics through chemical synthesis. **G. Boons***

11:30 – 398. Heparan sulfate mimetics: Promising therapeutics for a wide range of diseases. **V. Ferro***

11:45 – 399. Mouse inflammatory monocytes express SIGNR1 and differentiate into mature antigen presenting cells by uptake of oligomannose-coated liposomes. **Y. Matsuoka***, N. Kojima

Sheraton Waikiki
Kahuku

Bioorthogonal Chemistry: Tools and Applications in Chemical Biology (#343)

Organized by: J. Pezacki, Q. Lin, M. Finn, I. Hamachi, P. Chen
Presiding: P. Chen, I. Hamachi, Q. Lin, J. Pezacki

8:00 Welcome and Introductory Remarks

8:05 – 400. Bioorthogonal chemistry for biology and drug development. **C.R. Bertozzi**

8:45 – 401. Site-specific ADC generation using SMARTag™ technology. **D. Rabuka**

9:15 – 402. Metabolic labeling of polyisopilic acids in living primary hippocampal neurons by tissue-based system. **J. Choi***, K. Kang*, S. Joo*, I. Choi*

9:35 – 403. Novel tetrazine-mediated transfer reaction probes for turnover-amplified detection of biological nucleic acid targets. **B.T. Cisneros***, H. Wu, N.K. Devaraj

9:55 coffee break

10:10 – 404. Interfacial bioorthogonal chemistry based on tetrazine ligation with trans-cycloalkenes. **J. Fox***

10:50 – 405. Identifying prostate cancer biomarkers by profiling glycoproteins in human prostate tissue. **D. Spicciarich**, S.L. Maund, S.C. Purcell, D.M. Peehl, C.R. Bertozzi*

11:10 – 406. Transition-metal-mediated uncaging in living human cells – an emerging alternative to photolabile protecting groups. **T. Völker**, E. Meggers*

11:30 – 407. Bioorthogonal elimination reaction-mediated protein decaging in living cells. **P. Chen***

Sheraton Waikiki
Molokai

Small Molecule Interactions in Biomembranes (#418)

Organized by: M. Murata, M. Burke, J. Yu
Presiding: J. Yu

8:00 – 408. Making molecular prosthetics from membrane-active small molecules. **M. Burke***

8:40 – 409. Small molecule interactions with membrane sterols. **N. Matsumori**, Y. Umegawa, Y. Nakagawa, R. Espiritu, M. Murata

9:20 – 410. Phospholipid and sterol interactions by solid-state NMR: Roles in blood clotting and antifungal drug mechanisms. **C.M. Rienstra***

10:00 – 411. Molecular aspects of Amphoterin B mode of action. **M. Baginski***

10:40 – 412. Head group-selective interaction of cations and sugars with phospholipids in multiple component bilayer systems. **S. Matsuoka***

11:00 – 413. Design, synthesis, and biological evaluation of fluorinated baflomycin analogs as an NMR probe to analyze the interaction with vacuolar-type ATPase. **H. Tsuchikawa**, H. Shibata, T. Hayashi, S. Hanashima, N. Matsumori, M. Murata*, T. Usui

11:20 – 414. Mycolactone, a membrane perturbing bacterial toxin, behaves as a linocactant. C. Lopez, B. Swanson, J. Swanson, **G. Gnanakaran**

11:40 – 415. Structure and function of heronamides, polycyclic macrolactams from marine-derived actinomycetes. **S. Nishimura**, R. Sugiyama, K. Fujita, S. Ito, K. Sakanishi, Y. Iwabuchi, N. Kanoh, N. Matsumori, H. Kakeya

Thursday Afternoon

Sheraton Waikiki
Kohala/Kona

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly, A. Smith, H. Suga, V. Nanda, J. Huang, K. Kudo, R. Cheng, P. Lyu
Presiding: H. Suga

13:00 – 416. Rapid way for the discovery of macrocyclic peptide drug leads. **H. Suga***

13:30 – 417. In vitro selection for a cocrystallization ligand of a eukaryotic P-glycoprotein homolog. **C.J. Hipolito**, A. Kodan, T. Yamaguchi, Y. Kimura, K. Ueda, H. Kato, H. Suga*

13:50 – 418. Structural diversity of catalytic antibody light chains (Antigenases) and the solving method. **T. Uda**, S. Matsumoto, H. NAKASHIMA, S. Itou, E. Hifumi*

14:10 – 419. Cryptand library construction via the 10BASE_j-T for specific binding toward a cancer-related protein. **M. Kazuto**, **M. Taki***

14:30 – 420. Application of selenopeptides as the active-site models of selenoenzymes. **M. Iwaoka**

14:50 – 421. Development of selective peptide catalysts having secondary structures. **K. Kudo***, K. Akagawa

15:20 – 422. Unrecognized amidation reactivity of propargyl esters and its biological applications. **K.K. Vong**, K. Tanaka*

15:40 – 423. Identification and characterization of human sORF-encoded polypeptides. **A. Saghatelian**

16:10 – 424. Circular permutation: Database, prediction, and design. **P. Lyu***

16:40 – 425. Site-specific investigation of O-GlcNAc modifications using synthetic proteins. **M.R. Pratt**

17:00 – 426. Synthesis of sulfotyrosine containing peptides by incorporating fluoresfated tyrosine using an Fmoc solid-phase strategy. **j.w. kelly***, W. Chen, j. dong, K.B. Sharpless

Royal Hawaiian
Regency II

New Platforms for Natural Products Discovery (#18)

Organized by: G. Carter, R. Andersen, B. Copp, S. Matsunaga
Presiding: R. Andersen

13:00 – 427. Discovery and biological characterization of natural products with potent cytotoxicity against non-small cell lung cancer. **J.B. MacMillan***, D. Colosimo, N. Oswald

13:35 – 428. Microbial biodiscovery: Valuing the new, the known, the broken and the unknown. **R.J. Capon***

14:10 – 429. From marine toxins to promising anticancer agents through mechanistic insight and medicinal chemistry. **H. Luesch**

14:45 Break

15:15 – 430. Synthesis of the natural product marthiapeptide A: A complex heterocyclic containing macrocycle. **s.r. mcalpine***, Y. Zhang, A. Islam

15:50 – 431. Potentiating the activities of monoclonal antibodies for cancer and inflammatory disease treatment. **P. Senter**

16:25 – 432. Chemical and biochemical studies of alkaloids from marine invertebrates. **T.F. Molinski***

Sheraton Waikiki
Ewa

Characterization and Applications of Food Enzymes (#59)

Organized by: F. Chen, F. Chen, H. Ni, Y. Lee
Presiding: F. Chen, B.J. Savary, J. Wu

13:00 Introductory Remarks

13:05 – 433. Enzymology, structural characterization, and emerging applications of the thermally-tolerant *Citrus* fruit pectin methylesterase. **B. Savary***, J.C. Tovar, P. Vasu, R. Cameron

13:35 – 434. Application of proteases in preparing bioactive peptides. **J. Wu***

13:55 – 435. cDNA cloning of β -glucosidase gene from *Tricholoma matsutake*. **H. Onuma***, Y. Fukuta, M. Kusuda, T. Terashita, N. Shirasaka

14:15 – 436. Biochemical characterization of an intracellular 6 G-fructofuranosidase from *Xanthophyllomyces dendrophorus* and its application in production of neo-fructooligosaccharides (neo-FOSs). **P. Wang***, X. Xu, J. Chen, Z. Jin

14:35 – 437. Free astaxanthin preparation by lipase/astaxanthin esterase co-hydrolysis of its esters from *Haematococcus pluvialis* oil. **X. Mao***, H. Dong, C. Xue

14:55 Session Break

15:05 – 438. Biochemical characterization of two novel chitinases from *Paenibacillus barenzolzii* suitable for the production of N-acetyl glucosamine and N-acetyl chitobiose. **Z. Jiang**

15:35 – 439. Enzymatic synthesis of dipeptidyl prolyl-cyclic using L-amino acid esterase. **T. Tanaka***, M. Wakayama

15:55 – 440. Endogenous proteases and their inhibitors during autolysis of sea cucumber *Stichopus japonicus*. **L. Sun***, B. Zhu*, M. Yu, Y. Ma, H. Hou, G. Zhang

16:15 – 441. Internal amino-acid sequence of pigment from *Pleurotus salmonostrammeus*. **Y. Fujii**, Y. Fukuta, N. Shirasaka

16:35 – 442. Laccase: Fermentation process intensification and purification by functional magnetic nanoparticles. **C. Liu***

Sheraton Waikiki
Kauai

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

Organized by: Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang
Presiding: H. Lin

13:00 – 443. Reversible RNA and DNA methylation in gene expression regulation. **C. He**

13:30 – 444. Chemical technology for analysis of DNA epigenetic modification. **A. Okamoto***

14:00 – 445. Toward small-molecule non-nucleic acids inhibitors of DNA methyltransferases. **A. Gagnon***

14:30 – 446. Selective inhibition of EZH2 by EPZ-6438 as personalized cancer therapy. **T. Owa***

15:00 Break

15:10 – 447. Regulation of the core pre-mRNA splicing machinery by MYC and PRMT5 is essential to sustain lymphomagenesis. **E. GUCCIONE**

15:40 – 448. Discovery of selective protein arginine methyltransferase 5 (PRMT5) inhibitors and biological evaluations. **S. Yang**

16:10 – 449. OH-seq: A new method to produce a whole-genome map of chromosome topography. **T. Tullius**, C. Chiang, S.C. Parker

16:40 – 450. Design and synthesis of peptide probes for polycomb group proteins upregulated in stem cells and prostate cancer. **N.H. Milosevich***, M. Gignac, C. Simhadri, N. Prashar, R. Flemmer, J. Li, C. Croft, L. Bai, R. Kratofil, F. Hof

Royal Hawaiian
Regency III

Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

Organized by: M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada
Presiding: M. Ikura

13:00 – 451. Conformational dynamics in protein function: Comparisons of mesophilic and thermophilic ribonuclease H enzymes. **A.G. Palmer***

13:30 – 452. Large-amplitude, slow breathing motions in proteins: New insights for the dynamics of protein interiors and protein-ligand interfaces. **M. Kainosho**

14:00 – 453. Are intrinsically disordered protein termini important to biological function: Real or imaginary? **B.D. Sykes**

14:30 – 454. Direct observation of hierarchical protein dynamics. **J. Lewandowski, M. Halse, M. Blackledge, L. Emsley**

14:45 BREAK

15:00 – 455. Structural basis for antibody recognition of an intrinsically disordered antigen. **R.S. Norton**

15:30 – 456. Structural dynamics and their functional implications of the intrinsically disordered regions (IDRs) in transcription regulatory proteins. **S. Tate**

16:00 – 457. NMR characterization of dynamic conformational ensembles and interactions of carbohydrate chains. **K. Kato***

16:30 – 458. High fidelity protein dynamic properties analysis using nuclear magnetic resonance. **C. Tian***, Y. Xiong

16:45 – 459. Slow conformational switch in a dynamic transactivation domain regulates the 24-hour circadian clock. **C.L. Partch***

Royal Hawaiian
Regency I

Enzyme Engineering and Biocatalysis Applications (#222)

Organized by: J. Pelletier, S. Lutz, B. Kim, R. Kazlauskas, N. Itoh
Presiding: B. Kim

13:00 – 460. Development of enzyme-loaded polymeric nanocapsules as a versatile platform for enzyme applications: Effect of co-encapsulation of neutral macromolecules. **Y. Sakamura, H. Tang, T. Mori, Y. Katayama, A. Kishimura***

13:20 – 461. Engineering the dynamics in enzymes for reducing the product inhibition by facilitating the product release. **H. Kim***

14:00 – 462. Methyltransferase engineering: Using substrate analogs to turn alkylators into oxidizers. **K.C. Catcott***, Z. Zhou

* Principle Author

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14:20 – 463. Directed-ish evolution: Engineering bacterial nitroreductases as tools for cancer gene therapy and cell biology. E. Williams, J. Copp, R. Little, A. Patterson, J. Smail, J. Mumm, D. Ackerley*

14:40 COFFEE BREAK

14:50 – 464. Making biorefineries more cost-effective by on-site enzyme production. B.K. Ahring*

15:10 – 465. Progress toward a near-universal optogenetic activation strategy based on genetically "caged" proteins. R.E. Campbell*

15:50 – 466. Robust NAD(P)H regenerators for biotransformation. M. Hayashi*, H. Yamamoto

16:10 – 467. Recombinant myriococcum thermophilum cellobiose dehydrogenase possessing increased oxygen reactivity: Application in antimicrobial composites. G. Tegl*, B. Thallinger, B. Beer, C. Sigmund, R. Ludwig, G.S. Nyamhongo, G.M. Guebitz

Sheraton Waikiki
Lanai

Carbohydrate Recognition in Health and Disease (#342)

Organized by: G. Boons, Y. Ito, A. Demchenko, D. Vocadlo

13:00 – 468. O-GlcNAc occurs cotranslationally to stabilize nascent polypeptides. Y. Zhu, T. Liu, S. Cecioni, L. Eskandari, W. Zandberg, L. Willems, D.J. Vocadlo*

13:30 – 469. Targeting virus-host cell interactions for drug and vaccine discovery. M. von Itzstein

14:00 – 470. Carbocyclic carbohydrate mimics as inhibitors and inactivators of glycoside hydrolases. A. Bennett*, C. Adamson, R. Britton, S. Mohan

14:30 – 471. Effects of glycosylation on an immunodominant region of the HIV-1 envelope protein. J. Tian, C. Lopez, C. Derdeyn, B. Korber, G. Gnanakaran*

14:45 break

15:00 – 472. Exploring and exploiting carbohydrate-lectin interactions. X. Liu*

15:30 – 473. Probing specific cell-surface carbohydrate-protein interactions. S. Hung*

16:00 – 474. O-protecting groups in sialylation reactions: Scope and limitations. C. De Meo*

16:30 – 475. Stereoselective construction of challenging glycosidic linkages via anomeric O-alkylation. J. Zhu

Sheraton Waikiki
Kahuku

Bioorthogonal Chemistry: Tools and Applications in Chemical Biology (#343)

Organized by: J. Pezacki, Q. Lin, M. Finn, I. Hamachi, P. Chen
Presiding: P. Chen, I. Hamachi, Q. Lin, J. Pezacki

13:00 Introduction

13:05 – 476. Sugars and proteins: Toward a synthetic biology. B.G. Davis*

13:45 – 477. Optimizing the tetrazole-based photoclick chemistry for biological applications. Z. Yu, C.P. Ramil, T. Lewandowski, Q. Lin*

14:15 – 478. Template-assisted bioorthogonal photopolymerization of molecular glue for site-selective manipulation of biological events. J. Hatano*, K. Okuro*, T. Aida*

14:35 – 479. Acyl-acyl carrier protein synthetases: A versatile tool. K. Finzel, J. Beld, M. Burkart

14:55 Coffee Break

15:10 – 480. Site-specific labeling and cellular delivery of functional proteins. C.P. Hackenberger

15:50 – 481. Enzymatic protein modification using protein farnesyltransferase for biotechnology applications. M. Distefano, J.K. Dozier, M. Rashidian

16:10 – 482. Bioorthogonal CuAAC-based hemoglobin-hemoglobin coupling optimized by regioselective serial cross-linking. R. Kluger*, S. Singh

16:30 – 483. Diazo compounds: Versatile reagents for chemical biology and pharmacology. R.T. Raines*

Sheraton Waikiki
Molokai

Small Molecule Interactions in Biomembranes (#418)

Organized by: M. Murata, M. Burke, J. Yu
Presiding: M. Burke

13:00 – 484. Helix-loop-helix motif of amphipathic LK peptides as a nanomolar inhibitor of HIV-1 transcription. S. Jiang*, Y. Lee, M. Baba, J. Yu

13:20 – 485. Solid-state NMR investigations of membrane-curvature induction by viral proteins. M. Hong*, H. Yao, Y. Yang, T. Wang

14:00 – 486. Exploiting hemolytic amphiphilic peptides as a design template for cytotoxic antibody delivery. S. Futaki

14:40 – 487. Membrane permeability and ion transport across the cell membranes induced by binol-functionalized ion transporters. A. Hébert, A.R. Schmitz*

15:00 – 488. Interaction between transmembrane model peptides and ladder shaped polycyclic ethers (LSPs). K. Yamada, M. Satake*, S. Fukuzawa, K. Tachibana, M. Murata, T. Hara

15:20 – 489. Mechanism of self-assembly of a transmembrane pore triggered by specific biomembranes. K. Tanaka, J.M. Caaveiro, K. Morante, K. Tsumoto*

15:40 – 490. Study of synthetic membrane perturbing peptides incorporating crown-ether by oriented circular dichroism. P. Paquet-Côté*, J. Buerck, A. Ulrich, N. Voyer

16:00 – 491. Synergistic role of lipids and peptides in controlling membrane dynamics. E.G. Kelley, A.C. Woodka, M. Ohl, P.D. Butler, M. Nagao

16:20 – 492. Novel technique for forming supported anionic lipid membranes through vesicle fusion and an investigation of its interactions with chrysophycin-3. T.A. Camesen*, K. Wang, R. Nagarajan

16:40 – 493. Umbrella rotaxanes and their transmembrane transport properties: Transport of small anions and biological active macrocycles. J. Kempf, A.R. Schmitz*

Thursday Evening

Hawaii Convention Center
Halls I, II, III

New Platforms for Natural Products Discovery (#18)

Organized by: G. Carter, R. Andersen, B. Copp, S. Matsunaga
Presiding: G. Carter

Poster Session
19:00 – 21:00

494. Automated genomes-to-natural products platform. C. Johnston, M. Skinnider, M. Wyatt, X. Li, L. Yang, D. Zechel, B. Ma, N. Magarvey*

495. Basic research for the evaluation of novel apoptosis-inducing anti-tumor agent based on the binding inhibition of survivin and HBXIP. Y. Hasebe, T. Saitoh, T. Takamura, Y. Iida*

496. Investigation of the products of transformation of Stemodin analogs from *Beauveria bassiana* ATCC 7159 to generate an active site model of its cytochrome P450 enzyme. G.G. Williams*

497. New polyketides from dinoflagellate *Amphidinium* sp. T. Kubota*, T. Iwai, H. Sato, J. Kobayashi*

498. Construction of HAS2-GFP fusion vector for analysis of HAS2 intracellular localization. S. Tokioka, T. Ide, Y. Iida*

499. Elucidation of inhibition of apoptosis for the survivin-interaction with use of yeast two-hybrid method. T. Saitoh*, Y. Hasebe, T. Takamura, Y. Iida

500. Investigation of autolytic enzyme for antifungal agent. A. Kida, Y. Iida*

501. Study of fungal biotransformations on terpenoid substrates using alginate-immobilized filamentous fungi. M.A. Collins, P.B. Reese*

502. Goadsporin, a peptidic natural product which induces secondary metabolism in actinomycetes. T. Ozaki, S. Asamizu, H. Onaka*

503. Evaluation of the In vitro schistosomicidal activity of Brazilian ascidians. M.E. Ribeiro, J.P. Batista, L.G. Magalhães, G.M. Dias, M.L. Andrade e Silva, W.R. Cunha, P.M. Pauletti, V.H. Woolner, A.J. Singh, P.T. Northcote, A.H. Januario

504. Effect of endophytic fungal associations on the chemical profile of *Vochysia divaricata* seedlings. L.P. Pimenta, L.C. Kellner Filho, B.A. Soares Parpinelli, k.A. Siqueira, M.A. Soares, R.M. Costa, R.L. Tame Parreira, R.C. Sola Veneziani, M.L. Andrade e Silva, W.R. Cunha, P.M. Pauletti, A.H. Januario

505. Evaluation of hyaluronan production by HAS2 inducing compounds from *Atractylosides lanceae*. Y. Hosaka, Y. Iida*, Y. Nakamura, M. Naruoka

Characterization and Applications of Food Enzymes (#59)

Organized by: F. Chen, F. Chen, H. Ni, Y. Lee
Presiding: F. Chen

Poster Session
19:00 – 21:00

506. Extracellular production of recombinant *Bacillus deramificans* pullulanase in *Brevibacillus brevis*. X. Duan, C. Zou, J. Wu

507. Identification and analysis of antigenic epitopes of arginine kinase from *Scylla paramamosain*. L. Guang-Ming

508. Study on the enzyme related with GABA formation in *Lentinula edodes*. K. Iwamoto, Y. Fukuta, N. Shirasaka

509. Influence of probiotic fermentation on the efficacy components of fruit and vegetable. T. Xiong

510. Alkaline protease expressed by a recombinant strain and immobilization in microcapsules. S. Lin*, M. Zhang, R. Liang, J. Liu

511. Activation and conformational changes of mushroom polyphenoloxidase by high pressure microfluidization treatment. C. Liu*, W. Liu, J. Chen, J. Liu, Y. Yejun, J. Wan, W. Liu

512. Purification and cDNA cloning of β -xylosidase from *Tricholoma matsutake*. k. kamei*, Y. Fukuta, M. Kusuda, T. Terashita, N. Shirasaka

513. Purification and characterization of D-amino acid oxidases from *Aspergillus* sp. GI-3. A. Kariyone*, S. Yano, K. Takagi, M. Wakayama

514. Enhancing extracellular production of *Streptomyces* sp. FA1 xylanase by co-expression with phosphoperoxidase C. L. Su, J. Wu

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Kauai

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

Organized by: Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang
Presiding: M. Yoshida

19:00 – 515. CoREST in peace: Adventures in epigenetics drug discovery. P. Cole*, J.H. Kalin

19:30 – 516. Integrative chemical biology approaches to study histone post-translational modifications. X.D. Li*

19:55 – 517. SirT1ns and novel protein post-translational modifications. H. Lin*

20:20 – 518. New insights into protein acetylation from chemoproteomics. J.L. Meier

20:40 – 519. Bioorthogonal chemical probes of protein acetylation. Y. Zheng*

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Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

Organized by: M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada Presiding: G. Otting

19:00 – 520. Exploiting chemical shifts and RDCs in the study of structured and intrinsically disordered proteins. A. Bax*, Y. Shen, N. Sgourakis, A. Mantysyzov, J. Ying, J. Roche

19:30 – 521. Chemical tags for protein NMR spectroscopy. G. Otting*

20:00 – 522. PRE and PCS techniques utilized for high-resolution protein structure determination. C. Kojima*

20:15 – 523. NMR experiments for proteins at high-magnetic field strength. R. Ishima*

20:30 – 524. Study of cancer metabolism in real-time with Live NMR metabolomics. S. Park

20:45 – 525. Computational and experimental studies of CH and NH isotopic exchange effects on ^{13}C NMR spectra of small, rigid peptides. E.M. Kleist*, B. Hudson

Hawaii Convention Center
Halls I, II, III

Enzyme Engineering and Biocatalysis Applications (#222)

Organized by: J. Pelletier, S. Lutz, B. Kim, R. Kazlauskas, N. Itoh
Presiding: J. Pelletier

Poster Session
19:00 – 21:00

526. Super catalytic antibody light chains (Antigenase) capable of suppressing the infection of influenza virus. E. Hitomi*, T. Uda, M. Arakawa

527. Engineering a glucose-sensitive regulator. F. Wong*, K.J. Png, M.M. Zhang

528. Biocatalytic approach for enhancement of antimicrobial activity of 7,10-dihydroxy-8(E)-octadecenoic acid. I. Choi, H. Sohn, C. Hou, H. Kim*

529. Riboregulation of gene expression in *Synechococcus elongatus* PCC7942. D.T. Fox, M. Krishnamurthy, T. Kern, M.K. DeAgüero, S. Hennelly, T. Dale, S.N. Twary, S.R. Starkenburg, R. Martí-Arbona, K. Sanbonmatsu*, C. Unkefer

530. Modular multi-enzyme cascade reactions using highly stabilized enzyme microbeads. M. Gu*

531. Modeling of enhanced catalysis in multienzyme nanostructures: Effect of molecular scaffolds, spatial organization, and concentration. C. Chang*, C. Roberts

532. Creation of hypermultivalent protein polymer using horseradish peroxidase mediated tyrosol radical coupling reaction. K. Minamihata, S. Yamaguchi, K. Nakajima, T. Nagamune

533. Effect of hydrothermal dissolution on the rate of enzymatic hydrolysis. M. Kanna, Y. Fukutomi, Y. Matsumura

* Principle Author

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onlineprogram

- 534.** Efficient conversion of genomic promoter region by genome engineering systems. **W. Nomura***, H. Tamamura
- 535.** CorNet: Correlated mutation network analysis combined with structure and literature data to guide smart library design. **H. Joosten***
- 536.** Expression of a cloned alcohol oxidase gene from *Ochrobactrum* sp. AIU 033: Glyoxylate production from glycolate using resting cells of recombinant *Escherichia coli*. **M. Yamada***, H. Muto, K. Isobe
- 537.** Lipase-catalyzed stereoselective transesterification of 2-methylcycloalkanols. **K. Ashida**, C. Yamamoto, K. Hiraiwa, C. Fujiwara, Y. Utaka, T. Kitayama
- 538.** Thymidine phosphorylase synthesis of nucleosides labeled with three types of markers. **N. Terado**, A. Hatano
- 539.** Screening for cyclic dipeptide-producing fungi using enzymatic conversion by cyclo(Leu-Phe) oxidase. **M. Tokushima**, K. Takahashi, Y. Fukuda, T. Nitoda, H. Kanzaki*
- 540.** Identification and characterization of physiologically active γ -glutamyltranspeptidase in *Pseudomonas aeruginosa* PAO1. **M. Wakayama***, Y. Nonomura, K. Takagi, S. Yano
- 541.** Approach for an alignment of chaperonin GroEL complexes encapsulating metal nanoparticles. **H. Yoda**, O. Yamamoto, A. Koike-Takeshita*
- 542.** Expression and site-directed mutagenesis of the highly stable royal palm peroxidase in *Pitcairnia pastoana*. **H. Zhao***, Q.X. Li
- 543.** Inhibition studies of LL-diaminopimelate aminotransferases (Dapl). **E.M. Rodriguez-Lopez***, J.C. Vedera
- 544.** Quantification of free heme by using a sensor based on fluorescein-labeled heme oxygenase-1. Y. Nakashima, J. Taira, Y. Higashimoto, S. Sueda, H. Komatsu, **H. Sakamoto***
- 545.** Pros and cons between whole-cell microorganisms and Chiralscreen® in the quest of best biocatalyst for asymmetric reduction. R. Tsunekawa, N. Natori, M. Hataoka, **S. Sakurai**, K. Hanaya, M. Shoji, T. Sugai*
- 546.** Effect of alkyl tail length of allylic substrate analogs to the enantioselectivity of farnesyl pyrophosphate synthase from *Geobacillus stearothermophilus*. **P.Y. Samori**, Y. Yoshida, M. Kusakari, S. Murakami, B. Hatano, N. Ohya, T. Kijima
- 547.** Comparative study of transglycosylation and hydrolysis activities of β -glucosidases from different organisms. **S. Suganuma**, M. Terasaki, Y. Hayakawa, T. Nitoda, H. Kanzaki*
- 548.** Construction of cassette mutagenesis library for esterase containing GGGX-motif. **R. Momma**, S. Yoshida, N. Kawakami, K. Miyamoto
- 549.** Engineering increased activity of the key degradative enzyme chlorocatechol 1,2-dioxigenase from *Burkholderia xenovorans* LB400. **M. Muthu***, G. Lloyd Jones*
- 550.** High performance hybrid nano-cellulose design with the synergy effect-inactivity in cellulase activity between different CBD. **H. Nakazawa**, I. Okada, Y. Ishigaki, E. Kobayashi, M. Umetsu
- 551.** Recognition of remote stereogenic center in lipase-mediated kinetic resolution of 1,3-benzodioxoles, useful scaffold of chiral derivatizing reagents. **N. Natori**, M. Shoji, T. Sugai, K. Hanaya*
- 552.** Construction of GroEL-GFP protein which holds the chaperonin function: A tool to study elucidation of GroEL molecular mechanism in vivo. **Y. Nishimura**, T. Niwa, H. Taguchi, A. Koike-Takeshita*
- 553.** Detection of dopamine on glassy carbon electrode modified by using tyrosinase and multiwalled carbon nanotube. **D. Park***, S. Rahman*, H. Lee, S. Park, J. Park, G. Jeong, D. Kim
- 554.** Chemoenzymatic synthesis of blood group antigens and development of high-throughput assays enables a platform for screening blood group antigen-cleaving enzymes. **D. Kwan**, I. Constantinescu, R. Chapanian, M. Higgins, S. Ernst, M. Kotzler, E. Samain, A. Boraston, J. Kizhakkedathu, S.G. Withers*
- 555.** Structural basis for BVO substrate profile and stereospecificity. B. Yachnin, M. McEvoy, R. MacCushie, P. Lau, A. Berghuis
- 556.** Chemoenzymatic synthesis of epoxy-docosapentaenoic acids. **K. Lee**, J. Yang, L. Cheruzel, B. Hammock*, A. Lewis
- 557.** Expression of recombinant algal alcohol oxidase from *Trichoderma reesei*. **Y. Maegaki**, Y. Liu, K. Takeda, M. Yoshida, N. NAKAMURA, H. Ohno
- 558.** Screening of microorganisms from flowers for high reducing ability of the aldehyde group of oleuropein aglycon. **S. Makio**, T. Norimatsu, M. Jyo, K. Kikuchi, T. Nitoda, H. Kanzaki*
- 559.** Enzymatic removal of steryl glucosides from biodiesel. **H.G. Menzella**
- 560.** Characterizing the thioesterase from 6-deoxyerythronolide B synthase: Stereoselective macrolide and macrodiolide formation. **T.P. Hari***, A. Pinto, A.A. Caissie, C.N. Boddy
- 561.** Identification of phenylmalonate metabolic pathway in *Bordetella bronchiseptica* KU1201. **R. Hemmi***, S. Yoshida, N. Kawakami, K. Miyamoto
- 562.** Expansion of substrate scope of *Candida antarctica* lipase B toward bulky phenylalkanols by liquid carbon dioxide. **H.N. Hoang***, T. Matsuda
- 563.** Biochemical characterization of a novel xylanase from rhizosphere microorganisms. **M. Kanoh***, N. Kawakami, S. Yoshida, K. Miyamoto
- 564.** Genetic engineering of esterases to improve polyester hydrolysis. **K. Gitschler**, D. Ribitsch, S. Zittenbacher, E. Herrero Acero, K. Gruber, G.M. Guebitz*
- 565.** Biotransformation of flavonoid compounds using plant cultured cell. **Y. Fujitaka**, T. Akashi, S. Kawamura, T. Ono, K. Manabe, K. Ishihara, N. Nakajima, H. Hamada
- 566.** Screening of thermostable α -1,3-glucanase producing bacteria and characterization of the isolates. **H. Fujiki***, W. SUYOTHA, S. Yano, M. Wakayama
- 567.** Design of a potent host for artificial metal centers in asymmetric Diels-Alder reactions. **J. Fischer**, F. Quitterer, M. Groll, J. Eppinger*
- 568.** Enzymatic route to one-component thiol-alkene functional resins. **M. Finnveden**, S. Nameer, M. Johansson, M. Martinelle
- 569.** Proteins and oligopeptides as green catalysts for chiral epoxidations. **C. Béribié***, C. Bouchard, N. Voyer
- 570.** Biotransformation of stilbene compounds using plant cultured cells. **D. Uesugi**, E. Noyama, M. Araki, N. Nakayama, S. Okada, S. Ozaki, K. Shimoda, N. Kubota, H. Hamada
- 571.** Identification of novel cupredoxin homologs using overlapped conserved residues based approach. A. Goyal, K. Hwang, J. Kim*, S. Lee*
- 572.** Fluorescence-based kinetic assay for high-throughput discovery and engineering of stereoselective ω -transaminases. **H. Land***, T. Scheidt, M. Anderson, Y. Chen, P. Berglund, D. Yi, W. Fessner
- 573.** Glucose-driven chemo-mechanical autonomous drug-release system toward feedback control of blood glucose in diabetes. **R. XIE**, K. Kurihara, M. Munkhbayar, K. Toma, T. Arakawa, K. Mitsubayashi*
- 574.** Engineering of *Photobacterium Lipolyticum* M37 lipase to increase catalytic activity for efficient production of biodiesel. **K. Yang**, S. Jung, J. Lee, B. Sung, H. Kim, S. Kim
- 575.** Accurate detection and manipulation of adenylation domain functions in nonribosomal peptide synthetases by an enzyme-linked immunosorbent assay system using active site-directed probes for adenylation domains. **F. Ishikawa***, K. Miyamoto, S. Konno, S. Kasai, H. Kakeya*
- 576.** Enzymatic synthesis of chiral γ -amino acids Using ω -transaminase. **H. Yun**
- 577.** Synthesis of chitin/chitosan stereopolymers by phosphorylase-catalyzed enzymatic polymerization. **K. Yamashita**, R. Shimohigoshi, K. Yamamoto, J. Kadokawa*
- 578.** Development of biosensor system by degradation of azo dyes using azoreductase from *Geobacillus stearothermophilus*. **N. Suzuki***, T. Ooi, S. Murakami, B. Hatano, T. Kijima
- 579.** Investigating the sulfur incorporation mechanism into biotin. **D.L. Tran***, J.T. Jarrett
- 580.** Bioproduction of optically pure (S)-epoxides using styrene monoxygenase of *Rhodococcus* sp. ST-10 expressed in organic solvent-tolerant microorganism. **H. Toda**, N. Itoh*
- 581.** Design of an artificial cellulase with cellulose-binding DNA aptamer. **M. Takahara***, Y. Mori, G.A. Gonçalves, H. Nakazawa, M. Umetsu, N. Kamiya
- 582.** Characterizing and modifying archaeal prephenate dehydrogenases for efficient biocatalysis in tyrosine biosynthesis. **I. Shlaifer***, J.L. Turnbull*
- 583.** Isolation of bacterial expansins and enhancement of cellulose saccharification. **F. SUMISA***
- 584.** Asymmetric nitroaldol reactions of aromatic aldehydes using human serum albumin. **S. Asakura**, T. Shimoda, K. Matsumoto*
- 585.** Generation of functionally and structurally distinct *Rhizopus oryzae* lipase through protein folding memory. **A. Satomura**, K. Kuroda, M. Ueda
- 586.** Kaurene production in recombinant *Escherichia coli*. **P. Lee**, M. Kong
- 587.** Accelerated protein engineering using cell-free transcription-translation systems. **L.T. Quertinmont***, S. Lutz
- 588.** Ionic liquid-type activating agents for the lipase-catalyzed reaction. **T. Nishihara***, Y. Matsubara, Y. Fukaya, T. Nokami, T. Itoh
- 589.** Enzymatic production of dicarboxylic acids by combining an enzyme from *Phialomonium* sp. AIU 274 oxidizing the ω -amino group in ω -amino compounds and an aldehyde oxidase from *Pseudomonas* sp. AIU 362. **M. Ooe**, M. Yamada*, W. Hojo, T. Yamashita, K. Isobe
- 590.** Enhanced enantioselectivity of thermostable esterase from *Archaeoglobus fulgidus* toward (S)-ketoprofen ethyl ester using directed evolution and characterization of mutant esterases. **J. Kim***, E. Hong, H. Kang, Y. Ryu
- 591.** Screening of gene-specific amplicons from metagenomes for chiral biocatalysis. **M. Kazama**, S. Kariya, J. Kurokawa, H. Toda, N. Itoh*
- 592.** Ortho-hydroxylation of monophenolic compounds by tyrosinase. **B. Kim***, S. Lee, J. Lee
- 593.** Enzyme-mediated hydrolysis of aliphatic dicarboxylic acid diesters. **Y. Igawa**, H. Ise, S. Ichinoseki, A. Kobayashi, F. Maeda, K. Matsumoto*
- 594.** Facile dynamic kinetic resolution of amino acid esters in organic media by enzymatic hydrolysis combined with racemases from *Pseudomonas putida*. **T. Kijima***, K. Shimizu, S. Murakami, B. Hatano, N. Ohya
- 595.** Encapsulation of laccase and its biocatalysis in non-conventional media. **S. Kermasha***
- 596.** Biocatalyst activity of entomogenous fungi: Stereoselective reduction of carbonyl compounds using tochuksao and related species. **K. Ishihara**, G. Hori, N. Masuoka, H. Hamada, N. Nakajima
- 597.** Thiol-functionalization of oligo- and polysaccharides by phosphorylase-catalyzed enzymatic glycosylation. **T. Jodoi**, R. Shimohigoshi, K. Yamamoto, J. Kadokawa*
- 598.** Heterologous production and characterization of marine-derived tyrosinases in *E. coli*. **Y. Choi**
- 599.** Enzyme-assisted aqueous extraction of pumpkin oil. **G. Ustun**, **G. Balcioglu***, M. Tuter
- 600.** Preparation of chiral alcohols using actinobacteria: Biocatalyst activity of marine-derived actinomycetes. **K. Ishihara***, G. Hori, N. Masuoka, N. Nakajima, H. Hamada
- 601.** Biotransformation of monoterpenoids using plant cultured cell. **S. Doi**, S. Takara, J. Akahori, K. Shimoda, H. Hamada
- 602.** Cofactor-assisted protein folding in flavoenzymes. **S. Iamurri***, S. Lutz

Hawaii Convention Center
Halls I, II, III

Carbohydrate Recognition in Health and Disease (#342)

Organized by: G. Boons, Y. Ito, A. Demchenko, D. Vocadlo

Poster Session 19:00 - 21:00

- 603.** Hexavalent glycoclusters having tris-bipyridine ferrous complex cores for probing intramolecular carbohydrate-carbohydrate interactions. **Y. Nonaka**, T. Hasegawa*
- 604.** Synthesis and molecular recognition of ferrocene carrying two GlcNAc units. **F. Dai**, T. Hasegawa*
- 605.** Studies towards understanding the biosynthesis of the capsular polysaccharide in *Campylobacter jejuni*. **R.A. Ashmus**, A. Jayasuriya, C.Q. Wenzel, C.M. Szymanski, T. Lowary
- 606.** Probing interactions between cell wall binding proteins and *B. anthracis* secondary cell wall polysaccharide using synthetic compounds. **R.N. Chapman**, G. Boons*, L. Liu
- 607.** Design and synthesis of potential influenza viral neuraminidases inhibitors based on a fused cyclopropane scaffold. **C. Colombo**, A. Bennet*, M.B. Pinto, A. Bernardi
- 608.** Elucidation of the essential elements for recognition of anti-MUC1 antibodies. **F. García-Martin***, G. Artigas, E.J. Cabrita, H. Coelho, H. Hinou, C. Leclerc, R. Lo-Man, F. Marcelo, M. Takahiko, S. Nishimura
- 609.** Discovery, characterization, and exploitation of the first sulfoquinovosidase. **G. Speciale**, Y. Jin, G.J. Davies, S.J. Williams, **E.D. Goddard-Borger***
- 610.** Novel approach in cancer immunotherapy: Using synthetic α -gal epitope to increase the immunogenicity of tumor antigens. **L. Hao Sheng**, Y. Manabe, K. Tokunaga, N. Terao, S. Takamatsu, M. Tanemura, E. Miyoshi*, F. Koichi*
- 611.** Synthetic study of the polymer as multivalent bioprobe (V): Novel approach for lectin detection using combination of the glycocluster effect and FRET in the fluorogenic glycopolymers. **R. Hayama**, T. KOYAMA, K. Hatano, K. MATSUOKA*

* Principle Author

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<http://pacifichem.org/onlineprogram>

- 612.** Structural and functional evaluation of POMGnT1 modification using synthetic glycopeptide. **H. Hinou***, S. Kikuchi, A. Seo, S. Nishimura
- 613.** Computational modeling of carbohydrate recognition in norovirus capsid protein with Lewis antigen. **T. Ishida***, T. Kubota, H. Shirato
- 614.** Synthesis of substrate for analysis of hydrolysis reaction of ENGases. **N. Ishii**, C. Sunaga, Y. Yoshimura, J. Kumada, Y. Matsuzaki, I. Matsuo
- 615.** N-Glycosylation with synthetic undecaprenyl pyrophosphate-linked oligosaccharide to oligopeptides by PgIb oligosaccharidase from *Campylobacter jejuni*. **A. Ishiwata***, Y. Taguchi, Y. Lee, T. Watanabe, D. Kohda, Y. Ito
- 616.** High throughput evaluations of carbohydrate-carbohydrate interactions by using fluorescence intensity distribution analysis-polarization technique. **M. Iwamura**, T. Hasegawa*
- 617.** Chemical synthesis of ubiquitinated glycoproteins having different protein conformation. **M. Izumi***, H. Araki, M. Tominaga, R. Okamoto, Y. Kajihara
- 618.** Detection of *Helicobacter pylori* using carbohydrate conjugates. **J. Jeong**, S. Park, I. Shin*
- 619.** Suppression of IL-6 production from murine macrophages by phagocytosis mediated by the specific C-type lectin receptor. **Y. Kawachi**, N. Kojima*
- 620.** Synthetic lectin (SL) arrays to target tumor associated carbohydrate antigens (TACAs) for the detection and management of cancer. **J.J. Lavigne**
- 621.** Stereoselective synthesis of β -mannopyranosides in N-linked glycans. **X. Li***, H. Nguyen, J. Zhu
- 622.** Rare sugars as potential inducers of the rhamnose operon: Biotechnology and chemistry in the production of 6-deoxyhexoses and related monosaccharides. **Z. Liu***, C. Kelly, A. Yoshihara, K. Izumori, M. Wormald, J.M. Otero-Casas, A.M. Estevez-Reino, J. Heap, A. Kato, S. Jenkinson, G.W. Fleet, R.J. Estevez
- 623.** Synthesis and interactions of rhamnose iminosugar mimics with the rhamnose operon, rhamnosidases, and rhamnose isomerase. **Z. Liu***, C. Kelly, A. Yoshihara, K. Izumori, M. Wormald, J.M. Otero-Casas, A.M. Estevez-Reino, J. Heap, A. Kato, I. Adachi, S. Jenkinson, G.W. Fleet, R.J. Estevez
- 624.** Analysis of endo α -mannosidase using synthetic glycan. **I. Matsuo***, S. Iwamoto, Y. Yoshimura, N. Ishii, T. Utsui, A. Seko, Y. Takeda, Y. Ito
- 625.** Synthesis of helical glyco-polyacetylene for probing cation-induced carbohydrate-carbohydrate interactions. **R. Matsuoka**, T. Hasegawa*
- 626.** Molecular interaction between rhamnose and a bacteria recognition lectin. **S. Ng**, Y. Lee, T. Fu, T. Wu, S. Sue, T. Pai, M. Chang*
- 627.** Chemical synthesis of inducible co-stimulator molecule (ALIM/ICOS) bearing three complex-type oligosaccharides at the native positions. **H.M. NGUYEN**, M. Izumi, R. Okamoto, Y. Kajihara*
- 628.** Structure analysis of glycosaminoglycan-type oligosaccharides elongated on saccharide primers and investigation of their priming abilities. **Y. Otsuka***, T. Sato
- 629.** Synthesis of LacNAC derivatives used for identification of specific lectin binders. **C. Park**, I. Shin*
- 630.** Inhibition of rotavirus adhesion protein VP8 β utilizing asymmetric human milk oligosaccharides. **A. Prudden**, S. Wang, Z. Gao, L. Meng, K. Moremen, G. Boons*
- 631.** Targeting cancer's sweet spot: Taking advantage of a polymer platform. **Q. Qin***
- 632.** Complexation of PDI family protein ERp29 with lectin chaperone calreticulin. **M. Sakono***, A. Seko, Y. Takeda, Y. Ito
- 633.** Novel ionic glyco-tools to harness the glycosynthetic machinery of live systems. **I. Sittel***, M.C. Galan
- 634.** Glycation of bone matrix proteins and skeletal health. **G.E. Sroga***, A. Siddula, D. Vashishth

- 635.** Targeted labeling of glycans in B-cell lymphoma with CD22 ligands. **Y. Sun**, R. Xie, X. Chen*
- 636.** Linear synthesis and immunological evaluation of monoglycosylated and pentaglycosylated MUC1 vaccine candidates for cancer. **N.T. SUPEKAR**, A. Sirohiwal, S. Sarkar, M. Wolpert, G. Boons*
- 637.** Functional analysis of UDP-Glc: glycoprotein glucosyltransferase using synthetic substrates. **Y. Takeda**, A. Seko, K. Ohara, M. Hashisu, K. Fujikawa, N. Wang, Y. Ito*
- 638.** Synthetic study of Fc fragment by using Bio-SPPS and expression method. **M. Ueda**, S. Imada, R. Okamoto, M. Izumi, Y. Kajihara*
- 639.** Syntheses of LacdiNAc-containing trisaccharides applying for antibody discovering. **T. Utsui**, S. Miyazawa, N. Ishii, Y. Yoshimura, I. Matsuo
- 640.** Chemoenzymatic synthesis of homogeneous glycoproteins for studying glycan-mediated protein folding. **N. Wang***, A. Seko, Y. Takeda, Y. Ito*
- 641.** New family of 7-bladed bacterial family of lectins. P. Sykrova, J. Novotna, M. Pokorna, G. Demo, M. Wimmerova*
- 642.** Sialic acid-modified nucleic acids that bind to all kinds of influenza viruses. **M. Yamabe**, D. Akamatsu, K. Kaihatsu, N. Kato, Y. Ebata*
- 643.** Conformational dynamics of high-mannose-type oligosaccharides as studied by NMR spectroscopy combined with molecular dynamics simulation. **T. Yamaguchi***, T. Satoh, T. Zhu, K. Kato*
- 644.** Analysis for the mechanism of deposition and fibril formation of beta-amyloid on lipid membrane. **H. Yasumori**, T. Matsubara, R. Fukuda, N. Okawa, H. Hatsuta, M. Shigeo, A. Suzuki, K. Yanagisawa, T. Sato*
- 645.** Structural elucidation of fucosylated glycoepitopes: Nonconventional C-H $\bullet\bullet\bullet$ O hydrogen bonds contribute to a reduction of conformational flexibility. **M. Zierke**, T. Aeschbacher, M. Schubert*, B. Ernst*

Hawaii Convention Center Halls I, II, III

Bioorthogonal Chemistry: Tools and Applications in Chemical Biology (#343)

- Organized by:* J. Pezacki, Q. Lin, M. Finn, I. Hamachi, P. Chen
Presiding: P. Chen, I. Hamachi, Q. Lin, J. Pezacki
- Poster Session**
19:00 – 21:00
- 646.** Spontaneous reconstitution of functional transmembrane proteins during bioorthogonal phospholipid membrane synthesis. **C.M. Cole**, R.J. Brea, M. hardy, Y. Kim, J. Yang, N.K. Devaraj
- 647.** Expanding the bioorthogonal chemistry toolbox with click boronate formation. **B. Akgun**, S. Bernard, D. Hall*
- 648.** New methods for living virus labeling based on bioorthogonal chemistry. **H. XIE***, L. Huang, G. Lu
- 649.** In vivo imaging of sialic acid in a zebrafish cancer model. **N.A. Yee***, A. Baldridge, C.R. Bertozzi
- 650.** Azido-type selective reactions for molecular conjugation. **T. Hosoya***, S. Yoshida, A. Shirashi, K. Kanno, I. Kii, K. Johmoto, H. Uekusa, M. Hagiwara
- 651.** Construction of 3D tissues containing tubular structures by bioprinter. **T. Takamura**, M. Matusasaki, M. Akashi
- 652.** Development of CHAD-Linkers for theranostic multiplexed antibody constructs. **R.A. Willard-Charnley**, C.R. Bertozzi
- 653.** Development of histological evaluation method for the analysis of 3D tissues constructed by LBL technique. **A. Hiura**, M. Matusasaki, M. Akashi
- 654.** Electrochemical control of rapid bioorthogonal tetrazine ligations for selective functionalization of microelectrodes. **F. Ehret***, H. Wu, S.C. Alexander, N.K. Devaraj

- 655.** Exploration of novel methods for in situ vesicle formation and linking them with gene expression. **A. Bhattacharya***, N.K. Devaraj
- 656.** Fluorogenic RNA labeling facilitated by short encoded recognition sequences at the 3' end of transcribed RNAs. **S.C. Alexander*, K.N. Busby**, N.K. Devaraj
- 657.** In situ synthesis of fluorogenic bioorthogonal tetrazine probes and its application on bioorthogonal tetrazine-mediated transfer reactions facilitate reaction turnover in nucleic acid-templated detection of microRNA. **H. Wu**
- 658.** Isotope targeted glycoproteomics (Iso-Tag): A chemical proteomics platform for N- and O-glycopeptide discovery. **C. Woo***, C.R. Bertozzi, A. lavarone
- 659.** ppGalNAcT protein substrate identification: Bump-hole engineering and substrate delivery. **M.F. Debets***, L. Wagner*, M. Ito, C.R. Bertozzi
- 660.** Reassignment of a sense codon with unnatural amino acids. **T. Yoo***, B. Lee, S. Shin
- 661.** Substituted PABC linkers to improve the bioorthogonal activation rate and stability of prodrugs. **S. Matikonda***, F. Feidler, A.B. Gamble
- 662.** Transient protection of strained alkynes from click reaction via complexation with copper. **S. Yoshida***, Y. Hatakeyama, K. Johmoto, H. Uekusa, T. Hosoya*

Hawaii Convention Center
Halls I, II, III

Small Molecule Interactions in Biomembranes (#418)

Organized by: M. Murata, M. Burke, J. Yu
Presiding: M. Murata

Poster Session

- 663.** Physical interactions of catechin derivatives with cell membrane models. **T. Matsuzaiki***, H. Ito, V. Chevryeva, A. Makky, S. Kaufmann, M. Suganuma, S. Nakabayashi, H. Yoshikawa, M. Tanaka
- 664.** Relationship of accumulation pattern of amyloid β protein on lipid planar membrane with fibril morphology. **M. Iwamura**, T. Shimanouchi, S. Aoyagi, Y. Kimura
- 665.** Optimization and characterization of synthetic antimicrobial peptides. **N. Poulin**, G. Simon, P. Paquet-Côté, M. Auger, N. Voyer*
- 666.** Design and synthesis of tetracaine derivatives as CNG channel blockers. **S. Kirk***, J. Neal, C. Gangam, S. Wax, A. Andrade, K. Melich, J. Karpen
- 667.** The more the merrier: C-terminal multimerization potentiates membrane permeability of the prototypical cell penetrating peptide TatP. I. Monreal, **D.S. Dalisay**, G. Wayman, H. Aguilar, J.P. Saludes*
- 668.** Conjugation of methotrexate to cell penetrating peptide enhances anti-inflammatory effect of the drug. S. Hyun, Y. Choi, D. Kim, J. Ko, D. Chung*, J. Yu*
- 669.** Are mechanosensitive channels involved in entry of streptomycin in to the bacterial cell? **K. Hashimoto***, I. YABE, H. KAWASAKI
- 670.** Interactions of small molecules on mutant N-methyl-D-aspartate (NMDA) receptors: Implications for epilepsy. **B. Ito***, Y. Chen
- 671.** Susceptibility of the nAChR to inhibition is regulated by a single amino acid residue in the TM2 region. **E.K. Henze***, Y. Chen, J. Huang

Friday Morning

Sheraton Waikiki

Kohala/Kona

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly,

A. Smith, H. Suga, V. Nanda, J. Huang,

K. Kudo, R. Cheng, P. Lyu

Presiding: W. Lubell

8:00 – 672. Advances in the synthesis and application of heterocycle turn mimics. **W. Lubell**, N. Atmuri, M.K. Boukanoun, J. Dufour-Gallant, X. Hou, D. Chatenet, S. Chemtob

8:30 – 673. Synthetic, structural, and biological studies of peptides containing bulky dehydroamino acids. **S.L. Castle***

8:50 – 674. AApptides: From structure to function. **J. Cai**

9:10 – 675. Combinatorial library screening platform for rapid discovery and SAR of protein ligands. **K. Pels***, D. Trader, T. Kodadek

9:30 – 676. Optimization for robust and reliable high-throughput screening of bead-based peptide libraries. **J. Joe***, S. Lee, J. Lim, I. Gao, Y. Ong, J. Oon

9:50 Coffee Break

10:00 – 677. Flexible approaches for the selective C-terminal modification of peptides. **P.E. Dawson***

10:30 – 678. Chemoselective Staudinger reactions for the synthesis of functional peptide protein-conjugates. **C.P. Hackenberger***

10:50 – 679. New method for N-to-C directional peptide synthesis. **C.A. Hutton***, J.R. Cochrane, A. Pourvali

11:10 – 680. Sortase A as a tool for the enzymatic cyclization of disulfide-rich cyclic peptides. **D. Craik**, X. Jia, Y. Huang, L. Chan, J. Rosengren, C. Schroeder

Sheraton Waikiki

Molokai

Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10)

Organized by: S. Silverman, Z. Huang, Y. Li, Y. Lu, H. Suga

Presiding: Y. Li

8:00 Opening remarks

8:05 – 681. RNA mango: A fluorophore-binding aptamer for single molecule visualization of RNA and native RNA/protein complex purification. S. Jeng, **P.J. Unrau***, S. Pancharakshan

8:30 – 682. DNA nanotechnology-based dynamic organization on the nano-bio interfaces. **C. Fan**

8:55 – 683. Achieving room temperature DNA amplification by dialing in destabilization. **B. Alladin-Mustan***, J.M. Gibbs-Davis

9:15 – 684. Functional DNA nanotechnology: Precise spatial and dynamic controls of nanomaterials assembly and its applications in sensing, imaging, and targeted drug delivery. **Y. Lu***, L. Tan, J. Zhang, H. Xing

9:40 – 685. DNA nanostructures for cellular delivery of therapeutics. **H. Sleiman***

10:05 Break

* Principle Author

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- 10:20 – 686.** Toward the development of oligonucleotide-based therapeutic drugs. **M.J. Damha***
- 10:45 – 687.** Fine-tuning thermal stability and pH sensitivity of i-motif DNA structures. **R.M. Wadkins***, S.M. Reilly, R.K. Morgan, T.A. Brooks
- 11:05 – 688.** Selenium atom-specific functionalization for structure and function studies of nucleic acid–protein complexes. **R. Abdur**, J. Gan, J. Salom, **Z. Huang***
- 11:30 – 689.** Chemical biology of nucleic acids: DNA origami and artificial genetic switch. **H. Sugiyama***

Royal Hawaiian
Regency II

New Platforms for Natural Products Discovery (#18)

- Organized by:* G. Carter, R. Andersen, B. Copp, S. Matsunaga
Presiding: G. Carter
- 8:00 – 690.** Stimulation of secondary metabolism in actinomycetes. **B.A. Haltii**, F. Berre, A. Grunwald, L. Liang, N. Prigoda-Lee, E. McCauley, A. Sproule, R.G. Kerr*
- 8:35 – 691.** New methods for compound discovery in symbiosis. **E.W. Schmidt**
- 9:10 – 692.** Metagenome mining of sponge-derived natural products. **T. Wakimoto***
- 9:45 Break**
- 10:15 – 693.** Chemical diversity of limonoids from mangrove plants. **J. Wu***, L. Shen
- 10:50 – 694.** Genomes to natural products and back. **N. Magarvey***, M. Skinnider, G. Chen, C. Dejong, P. Rees
- 11:25 – 695.** Sponge-metabolomics for the discovery of new cytotoxic constituents. **K. Takada***

Hawaii Convention Center
Halls I, II, III

Biosynthesis of Natural Products (#27)

- Organized by:* I. Abe, B. Moore, D. Ro
- Poster Session**
10:00 – 12:00
- 696.** De novo biosynthesis of terminal alkyne-tagged natural products and applications. **W. Zhang***
- 697.** Functional and structural analysis of β -amino acid-activating adenylations enzymes in macrolactam biosynthesis. **A. Miyanaga***, J. Cieslak, Y. Shinohara, F. Kudo, T. Eguchi
- 698.** Elucidation of pseurotin biosynthetic pathway revealing the unexpected role of glutathione S-transferase in natural product biosynthesis. **Y. Tsunematsu***, T. Yamamoto, H. Noguchi, K. Hotta, K. Watanabe*
- 699.** Functional analysis of a new diterpene biosynthetic gene cluster in *Herpetosiphon aurantiacus*. **C. Nakano**, M. Oshima, N. Kurashima, T. Hoshino*
- 700.** Aspoquinolone biosynthesis: Non-heme dioxygenase catalyzes atypical oxidations of 6,7-bicycle to form 6,6-quinolone core of vindictin-type fungal alkaloid. **Y. Hirayama**, K. Watanabe*, N. Ishikawa, H. Noguchi, K. Hotta
- 701.** Understanding the role of ketoreductase in polyketide biosynthesis. **A. Garg**, D. Cane
- 702.** Oxidase domains in nonribosomal peptide synthesis: Probing the mechanism of thiazole and oxazole formation. **T.L. Schneider***, J.W. Dronzek
- 703.** Structure-function analyses of two novel plant type III polyketide synthases obtained from medicinal plant *Evodia rutaecarpa*. **T. Kodama***, T. Matsui, T. Mori, T. Tadokoshi, H. Noguchi, I. Abe, H. Morita*
- 704.** Synthetic plant activator affect production of antifungal compounds by fluorescent pseudomonads as biocontrol agent. **N. Akiyama**, K. Nara, N. Someya, T. Ikeda, T. Morohoshi

- 705.** Biosynthesis and characterization of the polyketide antibiotic 2,4-diacylphloroglucinol produced by plant-associated pseudomonads. **N. Ichimura***, T. Yamaguchi, T. Yokotsuka, K. Nara, N. Someya, T. Ikeda, T. Morohoshi*
- 706.** Enzymatic syntheses of unnatural head-to-tail pentacyclic triterpenes by sesquiterpene cyclase. **W. Okamoto**, **T. Sato**
- 707.** Cyclization of squalene from both termini: identification of an oncoceroid synthase and enzymatic synthesis of ambrein. **D. Ueda**, T. Hoshino, T. Sato
- 708.** Enzyme-catalyzed stereoselective intramolecular Diels-Alder reaction in biosynthesis of decalin-containing natural products. **M. Sato**, F. Yagishita, T. Mino, N. Uchiyama, A. Patel, Y. Chooi, Y. Goda, W. Xu, H. Noguchi, K. Hotta, K.N. Houk, Y. Tang, K. Watanabe*
- 709.** Biosynthetic study on fungal polyketides using *Aspergillus oryzae* heterologous expression system. **T. Ugai**, A. Minami, R. Fuji, H. Oguri, H. Oikawa*
- 710.** Characterization of PLP-dependent 3-aminoenzoate synthase PktV in pactamycin biosynthesis. **A. Hirayama**, A. Miyanaga, F. Kudo, T. Eguchi*
- 711.** Biosynthesis of antimycins with a reconstituted 3-formamidosalicylate pharmacophore in *Escherichia coli*. **J. Liu**, W. Zhang
- 712.** 1,3-Propanediol production from glycerol in engineered *K. pneumoniae* AJ4 by inactivating LPS biosynthesis-related *wabG* gene. **E. Hong***, J. Kim, S. Ha, H. Kang, Y. Hyu
- 713.** Functional identification of lycopene β -cyclase and β -carotene hydroxylase in a cyanobacterium *Arthrospira platensis*. **K. Sugiyama***, M. Ebisawa, Y. Nagashima, H. Suzuki, S. Takaichi, M. Yamada
- 714.** Substrate sequestration and protein-protein interactions of NRPS PCPs. **M.J. Jarekmo**, D. Lee, M. Burkart*
- 715.** Total biosynthetic study of antitumor antibiotic ophiobolins using Aspergillus oryzae heterologous expression system. **K. Narita***, R. Chiba, A. Minami, H. Oikawa
- 716.** New enzyme involved in the control of the stereochemistry in the decalin formation during equisetin biosynthesis. **N. Kato**, T. Nogawa, H. Hirota, S. Takahashi, J. Jang, J. Ahn, H. OSADA
- 717.** Detoxification catabolism of chlorophylls among a secondary plant Euglenophyceae: Physiology and biochemical processes. **J. Kawahara**, M. Maruyama, Y. Kashiyama*, T. Suzaku, A. Yokoyama, M. Nakazawa, T. Ishikawa, H. Tamaki
- 718.** Biosynthesis and efficient heterologous production of halianginic, the first marine myxobacterial polyketide antibiotic. **Y. Sun**, Z. Feng, T. Tsuge, J. Suh, **M. Ojika***
- 719.** Biosynthetic study of alkyl citrate natural products. I. Takeuchi*, A. Minami, H. Oikawa
- 720.** Engineering a tandem acyl carrier protein domain in 6-deoxyerythronolide B synthase. **Z. Wang**, C. Kim*
- 721.** Reconstitution of biosynthetic machinery for highly elaborated indole diterpene penitrem in *Aspergillus oryzae*.
- L. Chengwei**, K. Tagami, A. Minami, T. Matsumoto, H. Oikawa
- 722.** Rapid and efficient genome mining for novel fungal metabolite. **Y. Ye**, A. Minami, H. Oikawa
- 723.** Biosynthesis and characterization of the antibiotic phenazine-1-carboxylate produced by plant-associated *Pseudomonas chlororaphis* subsp. *aurantiaca*. **T. Morohoshi**, N. Someya, T. Ikeda
- 724.** Progress on chemoenzymatic total synthesis of albomycin δ_2 . **H. Kim***, J. An, W. Song
- 725.** Characterization of the first bryophyte isoprene synthase from the isoprene-emitting moss *Campylopus introflexus* (heath star moss). A.T. Lantz, J.F. Cardielo, T.A. Gee, M.G. Richards, T.N. Rosenstiel, A. Fisher*
- 726.** Improved astaxanthin productivity in *Haematococcus pluvialis* by fungicide. **J. Lee**, D. Vijayan, R. Praveenkumar, B. Kim, K. Lee, Y. Oh*
- 727.** Characterization of fatty acyl-CoA ligase for the biosynthesis of the extender unit of reveromycin A. **S. Takahashi**, T. Miyazawa, H. Osada
- 728.** Precursor-directed biosynthesis of unnatural novel alkaloids by using a plant type III polyketide synthase obtained from *Evodia rutaecarpa*. **T. Ito**, T. Kodama, H. Noguchi, I. Abe, H. Morita
- 729.** Study on solution structure of an acyl carrier protein domain from a highly reducing fungal iterative polyketide synthase and its interactions with an acyltransferase protein. **W. Xu***, Y. Tang
- 730.** Profiling of nonribosomal peptide synthetase activities using active site-directed proteomic probes for adenylation domains. **S. Konno**, F. Ishikawa*, T. Suzuki, N. Dohmae, H. Kakeya*
- 731.** Characterization of the unusual enzymatic transformations in cylindrocyclaphane biosynthesis. **H. Nakamura**, E.P. Balskus*
- 732.** Characterization of indole diterpene cytochrome genes in yeast. **m. tang**, Y. Tang
- 733.** Biosynthesis of the ortho-diazooxine secondary metabolite cremeomycin in *Streptomyces cremeus*. **Y. Sugai**, Y. Katsuyama, Y. Ohnishi*
- 734.** Exploring novel peptide ligase orthologs in *Actinobacteria*. **Y. Ogasawara***, J. Kawata, M. Noike, K. Furuhata, T. Dairi
- 735.** Exploring synthetic utility of natural product glycoside biosynthetic enzymes by genome mining, functional characterization, and combinatorial biosynthesis. **H. Chiu***
- 736.** Structure-function analyses of novel indole prenyltransferases. **T. Mori**, H. Morita, I. Abe*
- 737.** Functional identification of ζ -carotene isomerase (Z-ISO) in a cyanobacterium *Arthrospira platensis*. **K. Takahashi**, H. Fukuzumi, K. Shimizu, Y. Nagashima, H. Suzuki, S. Takaichi, M. Yamada, K. Sugiyama*
- 738.** Cloning of saprolignum biosynthetic gene cluster from *Streptomyces* sp. TK08046. **T. Kawasaki***, A. Moriyama, K. Nakagawa, N. Immura
- 739.** Biosynthesis of methanobactins. **H. Wang***

Sheraton Waikiki
Kauai

Frontiers in Chromatin Biology and Chemical Epigenetics/Epigenomics (#151)

Organized by: Y. Zheng, M. Yoshida, H. Lin, H. Jiang, A. Cheryl, Y. NAKAO, P. Cole, Y. Chang
Presiding: Y. Chang

- 8:00 – 745.** Development of chemical tools for imaging protein localization and epigenetic phenomena. **K. Kikuchi***
- 8:30 – 746.** Targeting PRMT5 for cancer therapeutics. **J. Park**, K. Qian, Y. Zheng, **K. Malik***

- 8:45 – 747.** Adipose stem cells: Potential for metabolic reprogramming. **S. Sugii**
- 9:20 – 748.** Direct lineage conversion of fibroblasts into oligodendrocyte progenitor cells. **J. Kim***, H. Lee*, M. Park, D. Nam, M. Araújo-Bravo, H. Zaehres

- 9:45 Break**
- 9:55 – 749.** Fluorescent smartprobes for live cell imaging. **M. Vendrell***

- 10:20 – 750.** Understanding cell probe, CDY1. **S. Park**, N. Kang, S. Yun, Y. Chang*
- 10:45 – 751.** Understanding the functional roles of histone methylation and acetylation. **S.D. Taverna***

- 11:10 – 752.** YcgC represents a new protein deacetylase family in prokaryote. **H. Zhu**
- 11:35 – 753.** Marine natural products that control a specific set of histone modifications. **D. Arai***, C. Sakuma, Y. Hayashi-Takanaka, H. Kimura, Y. Nakao

Royal Hawaiian
Regency III

Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

Organized by: M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada
Presiding: M. Tsai

- 8:00 – 754.** Hybrid methods approach to determine the structure of Tetrahymena telomerase. **J. Feigon***

- 8:30 – 755.** Structure and dynamics of the polymyxin-resistance-associated response regulator PrmrA in complex with the promoter DNA. **C. Chen***

- 9:00 – 756.** Molecular insight into the RanGTP level regulated by hMog1 for faithful mitotic chromosome segregation. **Y. Shi***

- 9:30 – 757.** NMR structural view and mechanism of non-Watson-Crick dG:dGTP incorporation by DNA polymerase X. **M. Tsai**

- 10:00 BREAK**
- 10:15 – 758.** Redefining the double helix using NMR. **H. Al-Hashimi***

- 10:45 – 759.** Structural and dynamics studies of the influenza A virus RNA and recognition mechanism by RIG-I. **B. Choi**

- 11:15 – 760.** Design of potent and selective integrin drugs for cancer. **W. Chuang***

- 11:45 – 761.** Structural mapping and comparability assessment of protein-based therapeutics using high-resolution NMR. **R.G. Brinson**, L.W. Arbogast, J.P. Marino*

* Principle Author

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Royal Hawaiian
Regency I

Enzyme Engineering and Biocatalysis Applications (#222)

Organized by: J. Pelletier, S. Lutz,
B. Kim, R. Kazlauskas, N. Itoh
Presiding: S. Lutz

8:00 – 762. Rapid evolution of enzymes for pharmaceutical applications.

J.J. Lalonde*, O. Alvizo, D. Entwistle

8:20 – 763. Dynamic amino acid networks regulate catalytic activity of tryptophan synthase. J. Axe, K. O'Rourke, N. Kerstetter, E. Yezdimer, D.D. Boehr*

8:40 – 764. Expanding the synthetic capabilities of yeast. V. Cornish

9:20 – 765. Ancestral α/β -hydrolases catalyze a broader range of reactions than the modern equivalents. T. Devamani, A. Rauwerdink, M. Lunzer, B. Jones, J. Mooney, M. Tan, Z. Zhang, J. Xu, A. Dean, R. Kazlauskas*

9:40 COFFEE BREAK

9:50 – 766. Indirect immobilization of cytochrome P450 and cofactor regeneration system on magnetic beads using PCNA subunit as a scaffolding protein.

T. Nagamune*, Y.C. Tan, H. Hirakawa

10:10 – 767. Engineering proteins for selective catalysis. H. Yang, C. Zhang, K. Ellis-Guardiola, P. Srivastava, J.C. Lewis

10:30 – 768. Metalloprotein design using genetic code expansion. L. Jiang, J. Wang

10:50 – 769. Enzymatic antifouling. J. Kim

Hawaii Convention Center
Halls I, II, III

Bioorganic Reaction Mechanisms (#224)

Organized by: J. Richard, M. Tanner, C. Easton

Poster Session 10:00 – 12:00

770. Effect of pressure and temperature on the viability and function of human-derived glioblastoma cell line a-172.

K. Ishikawa, A. Shimizu, B. yamanoha, K. Nei, S. Yamamoto

771. Structural study on reaction mechanisms of enzymes involved in resorcinol catabolism. Y. Hata*, T. Fujii, T. Yamauchi, T. Oikawa

772. Structure and mechanism of ObcA: An enzyme responsible for bacterial quorum sensing-dependent oxalogenesis.

S. RHEE*

773. Analysis of the stability of DNA duplexes containing DNA damages.

M. Suzuki, T. Kawada, M. Morikawa, T. Kobayashi, H. Miyazawa, K. Kino*

774. Rolling circle translation using small circular RNA. N. Abe*, Y. Nakano, H. Abe*

775. Coupling of polyaniline polymerization on giant vesicles with membrane fluctuation. T. Shimanouchi, S. Fukuma, P. Walde, Y. Kimura

776. Redox chemistry of the formylglycine-generating enzyme: A unique thiol oxidase. M.J. Appel, C.R. Bertozzi

777. Destabilization of a radical intermediate accelerates catalysis in a coenzyme B12-dependent aminomutase. C. Makins, G.A. DiLabio, K.R. Wolthers*

Sheraton Waikiki
Maui

Bio/chemical Approaches for Single Cell Biosensing Technologies (#257)

Organized by: E. Tamiya, K. Kerman, D. Chiu, G. Zhou

8:00 Opening remark

8:03 – 778. Toward innovative technology platforms for integrated single cell analysis. S. Sugano

8:23 – 779. Single cell omic analysis based on microfluidic chips. B. Liu*

8:38 – 780. Phosphorescence lifetime measurement for oxygen concentration imaging inside a single cel. T. Kamachi*, H. Ito, H. Kurokawa, M. Inoue, S. Yano, Y. Kobayashi

8:53 – 781. Ratiometric dual pH and oxygen intracellular sensors. F. Su*, K. Day, L. Zhang, X. Kong, Y. Tian, D.R. Meldrum

9:08 – 782. Imaging of single cancer and fungal cells using scanning electrochemical microscopy and multifunctional quantum dots. F. Zhou*, T. Kai*, G. Zhang, J. Lopez, J. Ren

9:23 – 783. Organotellurium probes for single cell multiparameter biology. L. Edgar, L. Willis, M. Nitiz

9:38 – 784. Enhanced-scRRBS for massive single cell methylome analysis toward *in silico* 3D-reconstructions of mouse and human tissues. J. Yamane, K. Kobayashi, N. Taniyama, W. FUJIBUCHI*

9:53 Coffee break

10:00 – 785. Signal amplification for bioanalysis and cytossensing. H. Ju

10:15 – 786. Microtechnologies to interrogate signaling in single cells.

N. Allbritton*

10:30 – 787. Membrane fluidity and cell signal transduction: Effect of menthol on cell membrane. M. TAKAGI*, S. YABUCHI, N. SHIMOKAWA, K. HOSHINO, Y. TSUJINO

10:45 – 788. Bioluminescence analysis in living cells using NanoLuc luciferase based probes. M. Hattori, T. Ozawa*

11:00 – 789. Development of Quenchbody to image and quantify tumor-associated membrane protein claudin. H. Ueda*, H. Jeong, T. Kawamura, M. Iida, Y. Kawahigashi, M. Takigawa, C. Chung, J. Dong, M. Kondoh

11:15 – 790. Decipherment of olfactory receptor repertoire by using an automated single-cell analysis and isolation system equipped with real-time calcium imaging device. N. Yoshimoto*, M. Suzuki, A. Kida, K. Shimono, S. Kuroda

11:30 – 791. Application of PC12 cells expressing Yellow Cameleon for monitoring the intracellular Ca^{2+} concentration change by nanosecond electric field stimulation. H. SHINOHARA*, M. SUGA, R. HASEGAWA

11:45 – 792. Droplet-based cell manipulation for analyzing environmental microbes at single-cell resolution. M. Hosokawa*, Y. Nishikawa, H. Takeyama

Sheraton Waikiki
Kahu

Bioorthogonal Chemistry: Tools and Applications in Chemical Biology (#343)

Organized by: J. Pezacki, Q. Lin, M. Finn, I. Hamachi, P. Chen

Presiding: P. Chen, I. Hamachi, Q. Lin, J. Pezacki

8:00 Introduction

8:05 – 793. Ligand-directed chemistry for bioorthogonal protein labeling in living system. I. Hamachi*

8:45 – 794. TO-ligation: A powerful tool for chemical biology. X. Lei*

9:15 – 795. Refined mechanism of the copper (I)-catalyzed azide–alkyne Huisgen cycloaddition reaction. W. Liu*

9:35 – 796. Bioorthogonal prodrug activation via a 1,3-dipolar cycloaddition.

A.B. Gamble*, S. Matikonda, D.L. Orsi, V. Staudacher, I.A. Jenkins, F. Feidler, J. Chen

9:55 Coffee Break

10:10 – 797. Chemoenzymatic methods for visualizing glycans in the immune system and human samples. P. Wu*

10:50 – 798. Visualizing mycobacterial trehalose glycolipids during infection.

F.P. Rodriguez-Rivera, C.R. Bertozzi*

11:10 – 799. Dual-intein autoprocessing domain that directs synchronized protein co-expression in both prokaryotes and eukaryotes. B. Zhang, M. Rapolu, Z. Liang, Z. Han, P.G. Williams, W. SU*

11:30 – 800. Strain-promoted alkyne-nitrene cycloaddition reactions and their use in studying host-pathogen interactions.

J. Pezacki*, A. Sherratt, M. Chigrinova, L. Cheung

Sheraton Waikiki
Honolulu

Chemistry and Applications of Retinal Proteins: From Microbes to Humans (#395)

Organized by: L. Brown, H. Kandori, M. Olivucci

Presiding: L. Brown

8:00 Introduction

8:05 – 801. Lessons from rhodopsin and bacteriorhodopsin: Engineered protein–chromophore systems with unique spectroscopic properties. B. Borhan*, J. Geiger

8:35 – 802. Understanding and designing color variants of retinal binding proteins by molecular simulations. S. Hayashi*

9:05 – 803. Proton transfers and water dynamics in retinal proteins. C. Mielack, A. Bondar*

9:35 – 804. Mechanistic insights from the crystal structure of an inward proton-transporting *Anabaena* sensory rhodopsin mutant. H. Luecke

9:50 – 805. Ultrafast 2D correlation spectroscopy elucidates primary proton pump dynamics in bacteriorhodopsin.

A. Yabushita*, C. Hung, C. Kao, C. Yang, T. Kobayashi

10:05 Break

10:15 – 806. Early activation of Channelrhodopsin-2: The EHT(E90-Helix2-Tilt)-model. K. Gerwert*

10:45 – 807. On the gating mechanism of channelrhodopsin. J. Heberle*

11:15 – 808. Spectroscopic and structural studies on the sodium transporting mechanism of sodium pump rhodopsin.

K. Inoue, H.E. Kato, Y. Kato, R. Abe-Yoshizumi, O. Nureki, H. Kandori*

11:30 – 809. Crystal structures of the N, X, and O states occurring in late steps of the ion pumping cycle of *pharaonis* halorhodopsin. T. Kouryama*

Hawaii Convention Center
Halls I, II, III

Biological General Posters

10:00 – 12:00

Agricultural and environmental biology

810. Effect of GABA-enriched brown rice on blood pressure in spontaneously hypertensive rats. K. Kawakami*, K. Yamada, T. Yamada, R. Takada, A. Sawabe, M. Nomura, T. Nabika

811. UPLC-MS analysis of endocannabinoids in plasma using magnetic dispersive micro-extraction (MDME). M. Guo*

812. Influence of food matrix on chemical properties and bio-activities of dry sugar-amino acid Maillard reaction models.

Y. Chen, X. Chen, D. Kitts

813. Isolation, identification, and characterization of lactic acid bacteria from raw milk and traditional food used for fermented dairy products. T. Kouya*, Y. Negoro

814. α -Glucosidase inhibitory effect of various coffees by three types extracting-methods. M. Shirahase, T. Furune, K. Terao, H. Yasui, Y. Yoshioka*

815. Physicochemical characteristics and toxicity of leachate from livestock mortality burial. J. Kim*, J. Choi, S. Han, J. Song, J. Park, C. Lee*

816. Effect of eggshell membrane on the inhibition of food discoloration. C. Maeta, M. Yamamura, Y. Nishio, S. Tabara, M. Tanaka, N. Konishi, N. Tanifujii

817. Extraordinary heat production of *Pseudomonas putida*. K. Tabata*, T. Kamachi

818. Changes of functional components and bacterial augmentation in the plastic-wrapped and vacuum packed fresh foods during cold storage. M. Moriyama*, R. Moriyama, A. Yamamoto, M. Kurotani

819. Functional characterization of chloride channel proteins in development of rice.

T. UM, G. JANG, Y. Choi*, S. CHANG, J. MOON

820. Inactivation of MS2 coliphage by UV and hydrogen peroxide: Comparison by cultural and molecular methodologies.

S.P. Sherchan*

821. Quality and antioxidant activity of ginseng seed processed by fermentation strains. K. Kim, M. LEE*, C. Cho, Y. RHEE, H. Hong, Y. LEE, Y. KIM, S. CHOI

822. Isolation and characterization of potassium-solubilizing bacteria and their status in rhizospheric microbial communities.

x. liu

823. Effect of the petit-high pressure carbon dioxide gas to the microbes. M. Kusube, R. Okabe, C. Horie, S. Hamada

Cancer therapy

824. Design and synthesis of a potent HDAC inhibitor. H. Jung*, C. Lee, J. Kim

825. Organometallic C \sim N-C(R) $_2$ C Au(III) coupled systems for cancer cell treatment.

S. Juergens*, F. Guarras, N. Ortiz*, F. Kuhn, A. Casini*

826. Antitumor activity of (-)-antofine via negative regulation of Met endosomal signaling in renal cancer cell. J. Song, Y. Kwon, S. Kim, S. Lee

827. Toxicity and mechanisms of transport of a novel organometallic Au(III) compound compared to cisplatin on rat kidney tissue slices ex vivo.

S. Spreckelmeyer*, G. Groothuis, I. Lambert, S. Stürup, C. Orwig, A. Casini

828. Gold-labeled liposomes enhances triggered drug release in tumor microenvironment by photothermal effect.

B.C. Shin*, S. Cho, H. Kwon

Peptides

829. (D-Trp) $_3$ -OMe: D-homo tripeptide constructed by enzymatic synthesis showed antibacterial activity against Gram-positive bacteria. Y. Isoda, Y. Tsunehara, J. Arima*

830. Effect of cell-penetrating peptides on interactions between liposomal membranes. T. Shimanouchi, M. Tanaka, P. Walde, D. Seebach, Y. Kimura

831. Construction of non-natural dipeptide library by peptide bond formation reaction catalyzed by D-stereospecific amidohydrolase. Y. Tsunehara, A. Tamura, Y. Isoda, J. Arima*

Bacteria and antimicrobials

832. Relationship of between biomembrane composition and fluidity. n. Iwamoto, K. Sumiyama, Y. Masaki, M. Kusube, M. Nishimoto

833. D-amino acid analogs to study the bacterial cell wall. P. Shieh, C.R. Bertozzi

834. Behavior of elongated *E.coli* membrane components under high pressure.

K. Sumiyama, M. Kusube

835. Piezophilic characterization of *Colwellia* MTCD1 from mariana trench challenger deep. K. Tanikawa, M. Kusube, D.H. Bartlett

836. Copper(II) complexes as antibiotic agents. D. Nguyen, N. Ng, M. Wu, J. Aldrich-Wright

* Principle Author

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Cell biology and biochemistry

837. Phosphorylations of Grb14 BPS domain by GSK-3 are correlated with complex forming between Grb14 and insulin receptor. **J. Taira***, Y. Higashimoto, H. Sakamoto

838. ATRX and small molecules bind to G-quadruplex formed by VNTR sequence and affect α -globin gene expression. **Y. Li**, J. Syed Jabarula, H. Sugiyama

839. Small molecular chemicals with botulinum toxin-like activity modulating neuro-exocytosis. **D. Kweon**, J. Park, Y. Jung, P. Heo

840. Design and development of a chemically-inducible activator of RAS. **J. Rose**, D. Maly

841. Analysis of chemoselective derivatives of carbonyl and thiol metabolites in complex mixtures by HRMS and NMR. **R.M. Higashi**, A.N. Lane, S. Gori, P. Lorkiewicz, S. Lauhle, N. Michael, S. Arumugam, H. Moseley, T.W. fan*

842. Exploring biomarker signatures of stress-associated diseases using ^1H NMR metabolomics. D. Kiss, E. Paxman, M. Ambeskovic, T. Montina, **G.A. Metz***

843. [Zn(hinokitiol)₂] complex showed the insulin-like effects on the insulin signaling pathway through an insulin-independent manner. **Y. Naito**, Y. Yoshikawa*, H. Yasui*, H. Yamamoto

844. Structural basis of PPAR γ transactivation by endocrine-disrupting organotin compounds. **T. Nakaniishi**, Y. Hiromori, S. Harada, S. Nakamura, S. Uchiyama, H. Nagase, T. Yoshida

Bioactive natural products

845. Probing the adhesion of *Caulobacter crescentus* holdfast by atomic force microscopy. **C. Berne***, M. Hernando-Pérez, X. Ma, N. Licata, B. Neves, S. Setayeshgar, Y. Brun, B. Dragnea

846. Anticancer activity of the flower bud of *Sophora japonica* L. through upregulating activating transcription factor 3 in human colorectal cancer cells. H. Jeong, J. Lee, G. Park, H. Eo, H. Song, M. Kim, J. Jeong

847. Sphingolipids upregulated caspase-14 expression by involvement of MAPK. **Y. Nagahara***, K. Kawakami, K. Sunaga

848. Anti-inflammatory and anti-proliferative activities of lees of Korean traditional rice wines. **S. Lee**, S. Woo, H. Sohn, W. Shin, J. Kim

849. Identification of natural product anti-cancers that inhibit CDC25c phosphatase activity. **K. Park**, H. Kang, S. Chung

850. Metabolomic analysis of protective effects of *Prunus mume* Sieb. et Zucc. on alcohol-induced liver injury by regulating apoptotic signaling pathway. **Y. Kim***, J. Pan, E. Lee, J. Lee

851. Identification novel natural product inhibitors for slingshot (SSH) family. **S. Lee**, Y. Lee, H. Kang, S. Chung

852. Effectivity of Citrus plants on lifestyle diseases: Anti-obesity effect of *Citrus unshiu* leaf. **K. Ito**, K. Shimizu, Y. Horikawa, N. Tomohiro, T. Tsutsumi, T. Hashizume, T. Fujita, M. Furuno, N. Utsunomiya, Y. Takada, T. Matsukawa, S. Kajiyama, Y. Nakagaki, A. Shimizu, K. Murata, H. Matsuda*

853. Effectiveness of sublingual immunotherapy with transgenic rice seeds expressing hypoallergenic modified antigens in murine allergic rhinitis model. **T. Yamada**, Y. Qu, F. Takaishi, N. Aoi, I. Morikura, T. Fuchiwaki, H. Kawachi

854. Effect of nutmeg (*Myristica fragrans* Houtt) on cedar pollinosis in mice. **H. Matsuo**, T. Yamada, K. Kawakami, R. Takeda, A. Sawabe, M. Nomura, T. Nabika

855. Lifestyle-related disease improvement effect of alpha-lipoic acid with γ -cyclodextrin. **Y. Hashimoto**, H. Okamoto, K. Terao, Y. Yoshikawa*

856. Discovery of potent natural product inhibitors for *Vaccinia* H1-related (VHR) phosphatase. **K. Roh**, H. Kang, S. Chung

857. Effects of saturated fatty acid to the lipid bilayer membrane fluidity. **Y. Masaki***, Y. Nishi, M. Kusube, M. Nishimoto

858. Effects of unsaturated fatty acid to lipid bilayer membrane fluidity. C. Nishikawa, Y. Masaki, **M. Nishimoto**

Enzymes and enzyme inhibitors

859. Family S9 peptidase from *Pleurotus eryngii*: Change in aminopeptidase function and substrate specificity by oxidation. **J. Arima***, S. Tokai, N. Mori

860. Cavity size of D-stereospecific amide-hydrolase relates to its side reaction "aminolysis". **K. Miyatani**, A. Ota, J. Arima*

861. Reductive dehalogenation reactions using modified cytochromes P450. **R.K. Bains***, J. Warren

862. trans-Aconitic acid from citric acid by whole-cell reactions of *Escherichia coli* heterologously expressing aconitase isomerase gene (*ais*). **K. Kobayashi**, K. Yuvara, H. Yonehara, J. Maruebi, T. Hattori, K. Kirimura

863. Characterization of the hot pepper (*Capsicum annuum*) NADPH-cytochrome P450 reductase. **Y. Jungs***, H. Kim, J. Kim, S. Park, S. Ma, C. Yun

864. Probing the binding orientation of endogenous substrate, epoxy-eicosanoid (EET), in soluble epoxide hydrolase with EET mimics. **K. Lee**, C.J. Ng, J. Yang, B. Hammock

865. Identification of mutations causing the increase in secretory laccase activity in agaricomycete *Coprinopsis cinerea*. **T. Nakazawa***, H. Muraguchi, Y. Honda

866. Distinct characteristics of two cys peroxiredoxins of *Vibrio vulnificus* suggesting differential roles in detoxifying oxidative stress. Y. Bang, M. Oh, **S. Choi***

Genes and transcription

867. Synthetic transcriptional activator of genes associated with retina in human dermal fibroblasts. **J. Syed Jabarulla**, A. Chandran, G. NAMASIVAYAM, J. Taniguchi, S. Sato, K. Hashiya, G. Kashiwazaki, T. Bando, H. Sugiyama*

868. Rational design of the specific binding hairpin Py-Im polyamides targeting human telomere sequences. **C. Guo***, Y. Kawamoto, S. Asamitsu, Y. Sawatani, K. Hashiya, T. Bando, H. Sugiyama*

869. Mixed isotope labeling strategies for biomarker analysis. **S.M. Lamos***

870. Identification of SNPs in genes that confer susceptibility to iron deficiency anemia and their potential association with the biochemical parameters of blood iron status and concentration among pregnant Filipinas. **V.A. Timoteo***, L.M. Dalmacio, M.V. Capanzana, J.S. Nacis, R.L. Agarrado

871. Synthetic genetic switches for directed differentiation of human pluripotent stem cells. **J. Taniguchi***, Y. Wei, T. Sadoi, S. Sato, G. NAMASIVAYAM, T. Bando, H. Sugiyama

872. Bioactivity of pyrrole-imidazole polyamides conjugated with a synthetic HAT activator. **G. Kashiwazaki***, G. NAMASIVAYAM, T. Bando, H. Sugiyama*

873. Effect of FABP2 Ala54Thr gene polymorphism on obesity and metabolic syndrome in Korean middle aged women with abdominal obesity. T. Han, **S. Woo***, Y. Kim

Proteins and protein structure

874. Purification and crystallization of a type II extradiol dioxygenase DesZ derived from *Spingobium* sp. SYK-6. **H. Matsubara**, N. Kamimura, E. Masai, T. Senda*

875. Volume fluctuation of protein in ionic liquid aqueous solutions at various temperatures. **K. Shimotani**, T. Inomata, K. Takayoshi, T. Kamiyama

876. Stability of protein in ionic liquids at various mole fraction. **M. Okabe**, T. Miki, K. Takayoshi, T. Kamiyama

877. Thermodynamic properties of sorbitol-induced molten globule state of myoglobin. **t. marutani**, T. Kamiyama, K. Takayoshi

878. Thermodynamic properties of aggregate state of proteins in dioxane aqueous solutions. **T. Kamiyama***, T. Inomata, K. Takayoshi

879. Altering stability of a transmembrane protein, MsbA, by structural comparison with its thermophilic homolog. **K. Lu***, T. Yamaguchi, T. Nakatsu, H. Kato

880. Copper-binding-induced tertiary folding of the cellular prion protein revealed by site-directed spin labeling with EPR spectroscopy and molecular dynamics. **J.M. Pushie**, E.G. Evans, G.L. Millhauser, G.N. George

881. Development of selective covalent labeling method for proteins and its application to visualization of proteins by transmission electron microscopy. **S. Tabata**, M. Kido, H. Fuchida, R. Shigemoto, I. Hamachi, A. Ojida*

882. Enhanced catalytic activity and oxidative stress tolerance in *Escherichia coli* by overexpression of Deinococcus Hsp20. **Y. Choi***

883. Selectivity of protein binding on surface templates of organosilane nanopatterns investigated using atomic force microscopy. **Z.L. Highland**, R. Girard, J.C. Ganno

884. Unnatural amino acids in proteins: Exploring the permissivity of orthogonal tRNA/aaRS pairs and designing biosensors. **L. Rowe***, B. Kelly, E. Wetzel, K. Puvar, R. Clark, T. Goyne

885. Fragment-based drug development targeting KEAP1/Nrf2 binding. **M. Zhong**, A. Lynch, S. Jehle, L. Luo, D. Kozakov, S. Vajda, K. Allen, A. Whitty

DNA and RNA

886. Identification of genomic targets of DNA binding small molecules using next generation sequencing. **A. Chandran**

R. Taylor, J. Syed Jabarulla, S. Sato, G. Kashiwazaki, T. Bando, H. Sugiyama*

887. DNA cleavage through reductive dioxygen activation by iron-bleomycin mimics. **A. Nomura***

888. Evaluating a molecular mechanism of the intracellular A-to-I RNA editing by analyzing a reaction behavior of ADAR2 in vitro and in the cell. **K. Nose**, A. Nishitarumizu, H. Umeno, H. Nakagawa, M. Deshimaru, M. Fukuda

889. Protein-dependent destabilization of DNA duplex on DNA-linked AuNP assembly. **Y. Kim***, X. Zheng, S. Park, H. Lee

890. Construction of artificial guide-RNAs for a site-directed RNA mutagenesis utilizing intracellular RNA editing by hADAR2. **H. Umeno**, A. Nishitarumizu, K. Nose, M. Deshimaru, M. Fukuda

891. Determining the efficacy of disinfectants against human noroviruses among 10 commercially available disinfectants in Asia. **M. Kim***, J. Choi, J. Kim

892. Studies of the rapid detection of *Staphylococcus aureus* by the antibody and isothermal target and probe amplification assay. **H. Shin***, G. Kang, J. Kim

893. Extra-chromosomal DNA maintenance in *Bacillus subtilis*, dependence on flagellation factor FlfF and moonlighting mediator EdmS. **Y. Hakumai***, k. shimomoto, M. Ashiuchi

894. Synthesis and evaluation of *N*-methyl-pyrrole-*N*-methylimidazole polyamide probes for human telomeres.

Y. Kawamoto*, A. Sasaki, S. Ide, K. Hashiya, T. Bando, K. Maeshima, H. Sugiyama*

895. Sequence-specific DNA alkylation and transcriptional inhibition by pyrrole-imidazole polyamide-chlorambucil conjugates. **S. Asamitsu**, Y. Kawamoto, F. Hashiya, K. Hashiya, M. Yamamoto, S. Kizaki, T. Bando*, H. Sugiyama*

Friday Afternoon

Sheraton Waikiki

Kohala/Kona

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly, A. Smith, H. Suga, V. Nanda, J. Huang, K. Kudo, R. Cheng, P. Lyu

Presiding: I. Smith

13:00 – 896. Understanding peptide macrocycles: From structural studies to oral bioavailability. **A.K. Yudin***

13:30 – 897. Comparing how heat shock protein inhibitors as oncogenic therapies: Have we forgotten something? **s.r. mcalpine**, Y. Wang

14:00 – 898. Preparation and preliminary biological evaluation of Ga-68 labeled somatostatin analog DOTA-Pasireotide. **F. Liu**, H. Zhu, X. Chliyi, C. Li, Z. Yang*

14:20 – 899. When structure leads to activity - analysis of a novel conotoxin. **N. Daly**, Z. Dekan, A. Jin, M. Smout, D. Wilson, A. Loukas, P. Alewood

14:50 – 900. Constrained peptide analogs elucidate the complex pharmacology of the Apelin GPCR. **R.C. Glen***, A.P. Davenport, J. Gavard, K.A. Jolliffe

15:10 – 901. Peptide isolated from the venom of bothrops asper enhances the activity of endothelin converting enzyme and neprilysin. **I. Smith***, S.D. Kuruppu

15:40 – 902. Modulating the apelin (APJ) receptor signaling with macrocycles. **E. Marsault***, A. Murza, É. Besserer-Offroy, J. Côté, J. Longpré, P. Sarret

16:00 – 903. Synthesis of a cytotoxic amitin for biorthogonal conjugation. **D. Perrin***, L. Zhao, D. Dietrich, A. Blanc, J. May, K. Matinkho, A. Pryma

16:30 – 904. Molecular recognition of venom peptides by acid-sensing ion channels and their therapeutic potential in stroke and pain. **L.D. Rash***

Royal Hawaiian Regency II

New Platforms for Natural Products Discovery (#18)

Organized by: G. Carter, R. Andersen, B. Copp, S. Matsunaga

Presiding: R. Andersen

13:00 – 905. Novel LXR antagonist represses hepatic steatosis and ameliorates glucose tolerance in mice. D. Won, J. Hong, E. Kim, J. Kim, T. Lee, H. Hwang, A. Giri, V. Reddy, D. Hahn, **H. Kang***

13:35 – 906. Genetic network analysis for target identification of theonellamides. **M. Yoshida***, S. Nishimura

14:10 – 907. Something old, something new, something bottled, something blue. **V.H. Woolner**, M. Stott, P.T. Northcote, **R.A. Keyzers***

14:45 Break

15:15 – 908. Bioprospecting in micro-algae: mega-scale meta-metabolomics. **G. Carter**

15:50 – 909. Phytochemical and biological investigations of *Conradina canescens* Gray. **N.S. Dosoky**, D.M. Moriarity, W.N. Setzer

16:25 – 910. Fungal fragments immobilized in calcium alginate: Transformation of substrates to new analogs. **P.C. Pearl**, A.R. Chen, **P.B. Reese***

Sheraton Waikiki
Kauai

Biosynthesis of Natural Products (#27)

Organized by: I. Abe, B. Moore, D. Ro

Presiding: B. Moore

* Principle Author

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13:00 – 911. Recent studies on fungal metabolite biosynthesis by iterative polyketide synthase enzymes.
J.C. Vedera*

13:30 – 912. Aspoquinolone biosynthesis: Non-heme dioxygenase catalyzes atypical oxidations of 6,7-bicyclic to form 6,6-quinolone core of viridicatin-type fungal alkaloid. **K. Watanabe***

14:00 – 913. Genome mining of filamentous fungi natural products. **Y. Tang**

14:30 – 914. Hapalindole alkaloid biosynthesis: a treasure trove of novel enzymatic transformations. **X. Liu***

14:50 – 915. Total biosynthetic study of bioactive fungal natural products: Pathway elucidation and genome mining.
H. Oikawa*

15:20 – 916. Discovery of novel natural products via synthetic biology. **H. Zhao**

15:50 – 917. Genome mining of natural product biosynthesis pathways in filamentous fungi. **C. Wang***

16:10 – 918. Cure for baldness and cryptic biosynthesis in *Streptomyces calvus*.
D. Zechel*

16:30 – 919. Diverse solutions in nature to the synthesis of beta-lactam antibiotics.
C.A. Townsend, J.M. Davidsen, D.H. Long, N.M. Gaudelli

Sheraton Waikiki
Ewa

Heat Shock Proteins: The Next Target in the Disease Frontier (#91)

Organized by: P. Wipf, S. McAlpine, P. Pan
Presiding: s.r. mcalpine, P. Wipf

13:00 – 920. Targeting protein-protein interactions in the heat shock protein 70 (Hsp70) complex. **J. Gestwicki***

13:40 – 921. 17-DIMAG induces HSP70 to ameliorate multiple organ dysfunction syndrome caused by endotoxemia in rats. **Y. Lee***

14:20 – 922. Hsp90 inhibitor drug conjugates (HDCs). **W. Ying***

15:00 – 923. Characterization and targeting of androgen receptor regulation by the Hsp90-associated cochaperone FKBP52 for the treatment of prostate cancer.
M.B. Cox

15:40 – 924. Developing HSP60/10 chaperonin inhibitors for breast cancer chemotherapy. **N. Salim, S.J. Abdeen, A. Ambrose, E. Chapman, S.M. Johnson***

16:10 Closing Remarks

Royal Hawaiian
Regency III

Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

Organized by: M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada
Presiding: W. Lee

13:00 – 925. Complex interactions among the proteins involved in the maturation of iron-sulfur proteins. **T.R. Alderson, J.H. Kim, J.L. Markley**

13:30 – 926. Structural aspects of gene regulation. **J. Mackay***, S. Webb, N. Shepherd, J. Low, A. Silva, D. Ryan

14:00 – 927. Allosteric inter-domain communication in protein kinase A. **M. Akimoto**, E.T. McNicholl, A. Ramkissoon, G. Melacini*

14:15 – 928. Look into the factors in modulating chemokine CXCL4 oligomerization. **Y. Chen, C. Lin, Y. Chen, C. Pan, S. Sue***

14:30 – 929. Structural basis of nonthermal plasma effect on cancer cells by NMR spectroscopy. **W. Lee***, S. Choi, P. Attri, E. Choi

15:00 BREAK

15:15 – 930. Cargo recognition mechanisms of unconventional myosins. **M. Zhang***

15:45 – 931. Self-mediated protein metamorphosis. **B. Xia***

16:15 – 932. Protein-protein interaction that involves coupled unfolding and binding.
J. Suh*

16:30 – 933. Structural polymorphism and substrate promiscuity a ribosome-associated molecular chaperone. **S. Hsu***, C. Huang, Y. Lai, Y. Chiang

16:45 – 934. Characterization of the functionally relevant changes in the structure and dynamics of PPIase. **J. Wang**, N. Tochio, Y. Tamari, R. Kawasaki, N. Xu, J. Uewaki, S. Tate

Royal Hawaiian
Regency I

Biorganic Reaction Mechanisms (#224)

Organized by: J. Richard, M. Tanner, C. Easton

Presiding: M.E. Tanner

13:00 – 935. Structural and mechanistic basis of capsular polysaccharide-synthesizing enzymes CapE/F, and the route to discovery novel inhibitors with antibacterial properties. **J.M. Caaveiro**, T. Miyafusa, T. Chigira, K. Nakano, S. Nagatohashi, K. Tsumoto*

13:20 – 936. Ring strain and mechanism-based inactivators. **A. Bennett**, M. Farren-Dai, N. Sannikova, T. Gloster

13:50 – 937. Inhibitors of enolase superfamily enzymes: Insights into evolution and active site architecture. **S. Bearne***, M. Nagar, B. Wyatt, M. St. Maurice, S. Aboushrawab

14:20 – 938. Getting bacteria to generate resistance inhibitors that lead to their own demise in the presence of antibiotics.
K. Auclair

14:55 – 939. Inhibition of resistance enzymes to rescue legacy antibiotics.
G. Wright*

15:30 – 940. Biomimetic approach to understanding inhibition of dihydropicolinic acid synthase. **D.R. Palmer***, D.A. Sanders, L. Konermann, Y. Skovpen, C. Conly, M. Sowole

16:00 – 941. Inhibition studies on cell shape-determining proteases and prenyltransferases. **Y. Liu, W. Abdelmagid, N. Mahmoodi, J. Morrison, M.E. Tanner***

16:30 – 942. Site-specific covalent post-translational modification of mRNA-displayed libraries for selection of peptide inhibitors. **S.A. Jongkees**, H. Suga

Sheraton Waikiki
Molokai

Bio/chemical Approaches for Single Cell Biosensing Technologies (#257)

Organized by: E. Tamiya, K. Kerman, D. Chiu, G. Zhou

13:00 – 943. Modified surfaces for capturing, monitoring the release of enzymes upon stimuli, and releasing cells down to the single cell level. **J. Gooding**, S.G. Parker, Y. Yang, Y. Zhu, B. Gupta, R. Piya, P.J. Reece, K. Gaus

13:20 – 944. High-resolution bioelectrochemical imaging and sensing for single cells. **T. Matsue**

13:35 – 945. NMR study on neurotransmitter diffusion in synaptic cleft using biomimetic extended-nanospaces. **Y. Kazoe***, Y. Tsuchiya, K. Mawatari, T. Kitamori

13:50 – 946. Molecular sensor to quantify the internalisation of nanoparticles and proteins. **A.P. Johnston***

14:05 – 947. High-resolution, quantitative analysis for measuring heterogeneities of G-protein signaling at single-cell levels in yeast. **J. Ishii***, A. Kondo

14:20 – 948. Nanoneedle technology for single cell biosensing and cell sorting.
C. Nakamura

14:35 – 949. Rapid and highly-effective formation of precise single-cell pairing based on dielectrophoresis.
T. YASUKAWA*, Y. Yoshimura, M. Tomita, F. Mizutani

14:50 Coffee break

14:57 – 950. Dual selection assay using circulating tumor cell subpopulations for precision medicine in cancer-related diseases. **S.A. Soper***

15:12 – 951. Integrated Smartphone quantum dot barcode device for diagnosing infected patients. **W.C. Chan***

15:27 – 952. In vitro sensing of cancer metastasis behaviors using 3D-vascular tissue models. **M. Matsusaki***, A. Nishiguchi, M. Akashi

15:42 – 953. In vitro 3D co-culture patterning model for evaluation of tumor cell malignancy. **M. OKOCHI***, Y. Shuhel, H. Honda

15:57 – 954. Development of neuron network high throughput screening device measuring single cell ionchannel current by planar patch clamp. **Z. Wang, H. Uno, T. Urisu***

16:12 – 955. Analysis of the intercellular communication in a pancreatic β cell cluster by microfluidic stimulation to single cell. **K. Terao***, K. Imai, T. Suzuki, H. Takao, F. Shimokawa, S. Matsuoaka, H. Kotera

16:27 – 956. Oligonucleotide synthesis on PDMS chip using mild reagents aiming to tag molecules in single cell analysis.
R. Bhardwaj, Y. Takamura*

16:42 – 957. Exploration of protein-ligand interactions by nm-ordered molecularly imprinted polymer thin layers containing specific ligands as interaction sites within the binding cavities. **Y. Kamon**, Y. Kitayama, T. Takeuchi*

16:57 Closing remark

Sheraton Waikiki
Kahuku

Bioorthogonal Chemistry: Tools and Applications in Chemical Biology (#343)

Organized by: J. Pezacki, Q. Lin, M. Finn, I. Hamachi, P. Chen

Presiding: P. Chen, I. Hamachi, Q. Lin, J. Pezacki

13:00 Introduction

13:05 – 958. Bioorthogonal modification of protein cages: From changing their biological function to applications in bio-nanotechnology. **J.J. Cornelissen**

13:45 – 959. Fluorogenic protein labelling.
J.W. Keillor*, Y. Chen, M. Strmiskova, C. Clouthier, K. Tsao

14:15 – 960. Toolbox of clickable and bioorthogonal gold nanoparticles: From synthesis to application. **P. Gobbo***, W. Luo, P. Gunawardene, S. Ghlassian, M. Workentin*

14:35 – 961. Systematic comparison of bioorthogonal reactions enables site-specific fluorescence labeling and imaging of intracellular proteins in live cells.
T. Peng*, H. Hang

14:55 Coffee break

15:10 – 962. Advancing bioorthogonal tetrazine reactions for applications in cellular imaging. **N.K. Devaraj**

15:50 – 963. Development of a cyanobenzothiazole-binding peptide tag for protein labeling. **S.G. Keyser**, C.R. Bertozzi*

16:10 – 964. SNAP-tag reactive lipid anchors enable targeted and spatiotemporally controlled localization of proteins to phospholipid membranes. **A. Rudd***, N.K. Devaraj

16:30 – 965. Photo-click chemistry tools for spatiotemporal control of reagentless ligation, labeling, immobilization, and cross-linking. **V. Popik**

Sheraton Waikiki
Honolulu

Chemistry and Applications of Retinal Proteins: From Microbes to Humans (#395)

Organized by: L. Brown, H. Kandori, M. Olivucci

Presiding: H. Kandori

13:00 Introduction

13:05 – 966. Microbial rhodopsins as multi-talented fluorescent reporters.
A.E. Cohen

13:35 – 967. Rhodopsin guanylyl cyclase of the aquatic fungus *Blastocladiella emersonii* enables fast optical control of cGMP signaling. **U. Scheibl**, K. Stehfest, C.E. Gee, H.G. Koerschen, R. Fudim, T. Oertner*, P. Hegemann*

13:50 – 968. Optogenetic silencing of neuronal activity using a light-driven sodium ion pump in marine bacteria. **T. Ishizuka**, S. Hososhima, M.R. Hoque, K. Yoshida, K. Inoue, H. Kandori, H. Yawo*

14:05 – 969. Mechanism diversity in microbial rhodopsins. **J.L. Spudich***

14:35 – 970. Characterization of new light-driven cation pumping rhodopsins and optogenetic application. **K. Jung**

14:50 – 971. Spectroscopic investigation of the red-activatable channelrhodopsin *ReaChR*. **B.S. Krause***, J. Kaufmann, F. Bartl, P. Hegemann

15:05 Break

15:15 – 972. From the structure of vertebrate and invertebrate rhodopsins to new applications in optogenetics. **G.F. Schertler***, E. Lesca, V. Pannels, X. Depu, R. Kammerer, R.J. Lucas, A. Terakita

15:45 – 973. Diverse animal bistable pigments and their optogenetic potential.
A. Terakita*

16:15 – 974. Evaluation of the spatial resolution and efficacy of a protein-based retinal implant. **N. Wagner***, J. Greco, R. Birge

16:30 – 975. Rhodopsin benchmarks novel chemical biology methods for single-molecule fluorescence imaging of GPCRs. **T. Huber**, T.P. Sakmar

16:45 – 976. Photochemical reaction cycle of *PsChR2* and its relationship to channel currents. **I. Szundi***, H. Li, E. Chen, R. Bogomolni, J.L. Spudich, D.S. Kliger*

Friday Evening

Hawaii Convention Center
Halls I, II, III

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly, A. Smith, H. Suga, V. Nanda, J. Huang, K. Kudo, R. Cheng, P. Lyu

Poster Session

19:00 – 21:00

977. Environmentally-responsive cyclic α,α -disubstituted α -amino acids for controlling peptide secondary structures.
M. Oba*, H. Nounaka, K. Furukawa, K. Toyama, M. Tanaka

978. Correlation and prognostic significance of mgmt promoter methylation and mgmt protein in glioblastomas. **T.V. Cao**

979. Artificial division of codon boxes to encode nonproteinogenic amino acids along with 20 proteinogenic ones.
Y. Iwane, A. Hitomi, H. Murakami, T. Katoh, Y. Goto, H. Suga*

980. High-speed *in vitro* display method for selection of functional peptides and proteins. **T. Ishizawa**, S. Nakayama, H. Murakami*

981. Molecular simulation of short selenopeptides by application of the SAAP force field. **N. Babe**, T. Suzuki, T. Shimosato, T. Minezaki, M. Iwaoka

982. Rapid purification of peptides and small proteins. **B. Kachel***, S. Jayanthi, T. Kumar

* Principle Author

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TECHNICAL PROGRAM

- 983.** Optical use of light for re-engineering protein function. **J. Lee***, J. Moon, J. Gam
- 984.** Antioxidant activity of short selenopeptides designed as glutathione peroxidase active-center models. **S. Shimodaira**, T. Takei, H. Hojo, M. Iwaoaka
- 985.** Photoinduced growth system of peptide nanofibers addressed by DNA hybridization photoinduced growth system of peptide nanofibers addressed by DNA hybridization. **A. Uemura**, M. Furutani, K. MATSUURA, A. Shigenaga, C. Komiyama, A. Otaka
- 986.** Global substrate specificity of serine hydrolases in *Mycobacterium smegmatis*. **B. Bassett***, R.J. Johnson
- 987.** Anti-aggregation effects on proteins during desiccation by model peptides of group-3 LEA proteins. **T. Furuki**, T. Shimizu, K. Yamakawa, R. Hatanaka, T. Takahashi, T. Kikawada, T. Okuda, H. Miura, A. Tunnicliffe, M. Sakurai*
- 988.** Effective synthesis and influenza virus inhibitory activities of carbosilane dendrimers peripherally functionalized with influenza hemagglutinin-binding peptide. **Y. Sato**, Y. Muramatsu, T. KOYAMA, K. MATSUOKA, R. Kuriyama, H. Kori, T. Matsubara, T. Sato, K. Hatano
- 989.** High cell penetrating ability and inducing apoptosis by conformationally constrained dimeric peptide at low concentration. **S. LEE**, S. Hyun, S. Kim, S. Jang, J. Yu*, Y. Lee*
- 990.** Parallel synthesis to construct a metal-chelating library as artificial metalloprotease candidates. **T. Midorikawa**, M. Taki*
- 991.** Antifusion effects on liposomes during desiccation by model peptides of group-3 LEA proteins. **T. Furuki**, M. Sakurai*
- 992.** Reinvestigation of oxidative folding pathways of bovine α -lactalbumin by using water-soluble selenium oxidant DH-SO_x. **R. Shinozaki***, M. Iwaoaka
- 993.** Protein conformational analysis by fluorescence-detected circular dichroism (FDCD). **T. Nehira***, **H. Ito**, K. Ishihara, K. Matsuo, S. Izumi, K. Ukena, K. Masuda, T. Yamazaki, A. Ishida
- 994.** Studies on lactam formation of arginine derivative using fluorous protecting group. **R. Akashi***
- 995.** Mechanistic investigations into the asymmetric epoxidation of enones catalyzed by 2,5-diketopiperazines. **C. Béribé***, X. Barbeau, P. Lagué, N. Voyer
- 996.** Role of the constant region of human antibody light chain for the structural diversity. **S. Itonaga**, T. Uda, E. Hifumi
- 997.** Thioester bond formation by ribosome and its application. **R. Takatsuji**, T. Katoh, H. Suga*
- 998.** Comparative atomic force microscopy (AFM) and field emission scanning electron microscopy (FE-SEM) studies of mixed phospholipid monolayers. **A. Sunda-Meya***, N. Phambu
- 999.** Efficient synthesis of hemoglobin-albumin cluster. **R. Funaki**, T. Komatsu*
- 1000.** Selective enrichment for hydroxyrosine-containing proteins toward proteomics. **M. Yanase**, G. Hayashi, A. Okamoto*
- 1001.** ScFv-ferritin as a novel targeted nanocage with high antigen-binding affinity. **H. Kang**, G. Go, S. Chung
- 1002.** Site-selective cleavage of target RNA by artificial RNA nucleases. **T. Mori**, K. Masaoka, Y. Fujita, R. Morisada, K. Sakabayashi, K. Mori, T. Tobimatsu, T. Sera*
- 1003.** Development of post-translational modification reactions for the synthesis of peptides with $\Psi(\text{CH}_2\text{NH})$ structures. **Y. Kato**, Y. Goto, H. Suga*
- 1004.** Three-days rapid construction of artificial antibody libraries on T7 bacteriophages. **Y. Saigusa**, M. Taki*
- 1005.** Enhanced function control of a multimeric protein by chemically designing one of its interfaces. **D. Sawada***, S. Sakurai, A. Tsuneshige
- 1006.** Optimization of surroundings of a solvatochromic fluorophore via the 10BASE_d-T for specific detection of a target protein. **H. Inoue**, M. Kazuto, Y. Arai, M. Taki*
- 1007.** Effects of calcium and lipids on recoverin, a neuronal calcium sensor (NCS) protein: Evidences from FTIR and solid-state NMR spectroscopy. **K. Potvin-Fournier**, A. Picard-Lafond, C. Marcotte, G. Valois-Paillard, T. Lefèvre, L. Cantin, C. Salesse, M. Auger
- 1008.** Synthesis and property of recombinant canine serum albumin. **K. Yamada***, R. Yoneyama, M. Akiyama, T. Komatsu*
- 1009.** Substrate multispecificity of a proton-coupled oligopeptide transporter, *Saccharomyces cerevisiae* Ptp2p. **K. Ito***, S. Kawai, T. Motoyama, Y. Yoshikawa, R. Kato, Y. Kawarasaki
- 1010.** Peptide-membrane interaction studies applied to Combi-2: effect of metal ions. **B. Almarwani**, A. Sunda-Meya, N. Phambu*
- 1011.** Recombinant production and purification of Interleukin-1 α using novel soluble affinity tag. **M.H. Al-Ameer***, S. Jayanthi, T. Kumar
- 1012.** Effects of an antimicrobial peptide on the biophysical properties of model membranes. **A.T. Alshammari**, A. Sunda-Meya, N. Phambu
- 1013.** Consensus-based approach to protein structure prediction. **B.E. Husic***, J. Ponder
- 1014.** Control of site-specific silica and calcium precipitation on DNA using a designed peptide. **M. Ozaki**, N. Endo, T. Imai, **K. Tomizaki**, K. Usui*
- 1015.** Fluorescence ratiometric detection of antigen using double fluorescent-labeled scFv based on FRET and fluorescence quenching. **K. Yoshikoshi***, T. Hoshika
- 1016.** Novel IgG-based fluorescent biosensor that shows antigen-dependent fluorescence enhancement. **K. Fukunaga**, T. Watanabe, D. Novitasari, T. Hoshika*
- 1017.** Incorporation of a photoisomerizable non-natural amino acid into proteins through *in vitro* and *in vivo* protein expression. **R. Shiba**, T. Watanabe, T. Hoshika*
- 1018.** Improvement of biological activities of syringolin A. **T. Chiba**, A. Matsuda, S. Ichikawa
- 1019.** Novel α helical peptide with membrane-disruptive properties for endosomal escape. **S. Nam**
- 1020.** Theoretical study on potency and selectivity of dipeptidyl peptidase IV inhibitors using the first-principles calculation. **S. Okazaki**, E. Ishitsubo, Y. Nakano, H. Shimano, H. TOKIWA*
- 1021.** Preparation of BSA-based hybrid enzyme containing multiple functions. **K. Hanaya***, S. Yamazawa, M. Shoji, T. Sugai
- 1022.** Genome editing in *Escherichia coli* by sandwiched zinc-finger nuclease. **T. Kai**, K. Shirimi, S. Ohno, T. Mori, K. Mori, T. Tobimatsu, T. Sera*
- 1023.** Structural analysis of RNA-binding protein to generate artificial RNA-binding proteins. **T. Nakao**, K. Nakamura, Y. Fujita, K. Masaoka, T. Mori, K. Mori, T. Tobimatsu, T. Sera*
- 1024.** Peptide-based tunable molecular wires. **G.M. Sylvia***, J. Horsley, J. Yu, A. Abel
- 1025.** Zinc-finger-based artificial transcription factors and their applications. **K. Ota**, N. Nishida, T. Mori, K. Mori, T. Tobimatsu, T. Sera*
- 1026.** Construction of self-assembled artificial viral capsid decorated with fab fragment. **Y. Shiomi**, T. Honjo, K. MATSUURA*
- 1027.** Immunoglobulin Fc-fused, neuropilin-1-specific peptide penetrates tumor tissue efficiently and inhibits tumor growth via anti-angiogenesis. **Y. Kim**, J. Bae, J. Kim, Y. Kim*
- 1028.** Photo-triggered fluorescent labeling of recombinant proteins in live cells. **Y. Kwon***
- 1029.** Quantification of proteins by selected reaction monitoring mass spectrometry. **S. Niwayama***, S. Kurono
- 1030.** Evaluation of cell-penetrating helical peptides having five-membered ring substituted amino acids. **T. Kato**, M. Oba, M. Tanaka
- 1031.** Thermodynamic analysis for the interaction between sugar-mimic peptide and hemagglutinin. **S. Yoshikawa***, T. Matsubara, T. Sato
- 1032.** Affinity selection of hemagglutinin-binding heptapeptide and *in silico* docking simulation. **T. Matsubara**, A. Onishi, D. Yamaguchi, T. Sato*
- 1033.** Design and construction of a novel heparin-binding peptide for the purification of recombinant proteins. **J.A. Morris**, S. Jayanthi, T. Kumar*
- 1034.** Development of FcBP-ferritin nanocage as a novel targeted delivery platform. **H. Kang**, G. Go, S. Chung
- 1035.** Protective effects on enzymes during desiccation by model peptides of group-3 LEA proteins. **T. Furuki**, M. Sakurai*
- 1036.** Chemical and biochemical features of human catalytic antibody light chain, #7 clone. **H. NAKASHIMA**, T. Uda, E. Hifumi
- 1037.** Synthesis of D, L-amino acid derivatives bearing thiol at the β -position and its enzymatic optical resolution. **Y. Morishita***
- 1038.** Peptide-based supramolecular structures. **B.R. Linton***
- 1039.** Selection and engineering design of short molecular binders recognizing biomarker proteins. **H. Hwang**, M. Ryu, J. Park*
- 1040.** Catalytic and anticancer functions of human super catalytic antibody (antigenase). **T. NONAKA**, T. Uda, E. Hifumi
- 1041.** Expression and refolding of the taste modifying plant protein, Miraculin. **S. Yamaguchi**, M. Namba, N. Hashikawa
- 1042.** O₂-affinity and safety of hemoglobin-albumin cluster. **H. Iwasaki**, R. Haruki, T. Komatsu*
- 1043.** Inclusion behavior of fluorescent molecules into artificial viral capsids self-assembled from β -annulus peptide. **S. Fujita**, K. MATSUURA*
- 1044.** Creation of artificial viral capsid modified oligohistidine chain. **T. Sakata**, T. Iwasaki, K. MATSUURA*

Sheraton Waikiki
Kauai

Biosynthesis of Natural Products (#27)

Organized by: I. Abe, B. Moore, D. Ro
Presiding: C.A. Townsend

19:00 – 1052. Biosynthesis of macrolactam antibiotics. **T. Eguchi***

19:30 – 1053. Engineered biosynthesis of glycosylated natural products. **Y. Yoon***

19:50 – 1054. Orthogonal mechanism to link sugars in the biosynthesis of antibiotic polysaccharides. **B.O. Bachmann***

20:10 – 1055. Biosynthesis and physiological function of a moss-specific diterpenoid hormone. **H. Kawaide***, S. Miyazaki, M. Nakajima

20:30 – 1056. Creating the Facebook for natural product analysis. **P. Dorrestein**

Hawaii Convention Center
Halls I, II, III

Heat Shock Proteins: The Next Target in the Disease Frontier (#91)

Organized by: P. Wipf, S. McAlpine, P. Pan

Poster Session

19:00 – 21:00

1057. Role of heat shock proteins in the protective effect of raloxifene in endotoxemic rats. **H.H. Shen**, Y. Lee

1058. 17-DMAG, an Hsp90 inhibitor, improves ovariectomy-induced obesity in female rats. **s. Leu***, Y. Tsai, P. Cheng

1059. Role of heat shock proteins on depression-like behavior in mice. **M. Ogawa***, T. Ogawa, Y. Utaka, N. Hashikawa-Hobara, N. Hashikawa

1060. The forgotten heat shock protein, HSP27: The design and synthesis of molecules targeting HSP27 as chemotherapies. **J. Kho**, R. Mehmood, H. Ecroyd, s.r. mcalpine*

1061. Crystal structure of a symmetric football-shaped GroEL:GroES₂:ATP₁₄ complex reveals rearrangement between two GroEL rings. **A. Koike-Takeshita***, T. Arakawa, H. Taguchi, T. Shimamura

Sheraton Waikiki
Molokai

Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

Organized by: M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada
Presiding: A.M. Gronenborn

19:00 – 1045. Triazole-linked analogs of DNA and RNA (¹T-DNA and ¹T-RNA): Synthesis and functions. **T. Fujino**, N. Yamazaki, K. Yasumoto, K. Endo, K. Okada, N. Tsunaka, A. Hasome, K. Sogawa, H. Isobe*

19:15 – 1046. RNA-aptamer probes for *in vivo* single virus assembly studies. **I.B. Tsvetkova***, G. Yi, C. Kao, B. Dragnea

19:30 – 1047. Site-specific regulation and maintenance of an expanded genetic alphabet. **B.M. Lamb**

19:45 – 1048. Synthesis of novel pseudouridine derivatives for the selective recognition of CG base pairs in triple-helix DNA. **H. Okamura**, Y. Taniguchi, S. Sasak*

20:00 – 1049. Improvements to prediction of RNA secondary structure from sequence. **B.M. Znosko***

20:15 – 1050. In vitro selection of new RNA-cleaving DNAAzymes, biochemical studies and analytical applications. **J. Liu***

20:30 – 1051. Synthesis and hybridization property of a boat-shaped pyranosyl nucleic acid analog whose nucleobase orientation is similar to that of natural RNA. **T. Kanagawa**, K. Mori, T. Kodama, S. Obika

* Principle Author

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- 20:15 – 1066.** Substrate-bound form of heat shock 70 kDa protein (HSP70) maintains the open lid structure in contrast to the X-ray structure. **N. Tochio**, M. Hoshikawa, S. Tate*
- 20:30 – 1067.** Revised structures of halogenated sucrose prepared using Appel reactions by one- and 2D magnetic resonance spectroscopy. **Z.P. Tachrim**, L. Wang, Y. Hashidoko, M. Hashimoto
- 20:45 – 1068.** NMR approach for biomedical application. **H. Takahashi***

Sheraton Waikiki
Waianae

Bioorganic Reaction Mechanisms (#224)

Organized by: J. Richard, M. Tanner,
C. Easton
Presiding: J. Richard

- 19:00 – 1069.** Six to five membered rings: Structural, mechanistic, and inhibition studies of novel sugar biosynthetic enzymes in pathogenic microorganisms. **D.A. Sanders**
- 19:20 – 1070.** Enzyme architecture: Optimization of transition state stabilization from a cation-phosphodianion pair. **J. Richard***, T.L. Amyes, A.C. Reyes
- 19:45 – 1071.** Unraveling the novel deoxy-nucleoside triphosphate triphosphohydrolase activity of the HIV restriction factor SAMHD1. **M. Webb**, I. Taylor, K. Bishop, D. Schwefel, V. Ennis Adeniran, G. Kelly, L. Arnold, D. Goldstone, H. Groom, S. Kunzelmann, J. Stoye
- 20:10 – 1072.** Theoretical study on a missing piece in understanding of biosynthesis of anthocyanin. **H. Sato***, C. WANG, K. Saito, M. Uchiyama
- 20:35 – 1073.** Toward isoform-specific lipid oxygenase inhibitors: Acetaminophen-inspired compounds. **R. Shah**, M. Haycock, D. Pratt*

Hawaii Convention Center
Halls I, II, III

Bio/chemical Approaches for Single Cell Biosensing Technologies (#257)

- Organized by: E. Tamiya, K. Kerman, D. Chiu, G. Zhou
Poster Session
19:00 – 21:00
- 1074.** New assay method of nephrotoxic chemicals using transparent transgenic zebrafish. **S. Akiyama***
- 1075.** Integrating reductive and synthetic approaches in biology using man-made cell-like compartments. **W. Aoki***, M. Saito, E. Tamiya*
- 1076.** Fabrication of single neural stem cell chip to detect cellular redox state based on spectroelectrochemical method. **J. Choi***, W. El-Said, T. Kim, Y. Chung
- 1077.** Cytogenetic effects of low-dose tritiated water in human peripheral blood lymphocytes. **B. Deng**, y. quan, z. tan
- 1078.** Isothermal and visual RNA detection system using enzymatic signal amplification and specific emission of thioflavin-T analog. **H. Fujita**, Y. Kataoka, M. Kuwahara*
- 1079.** Imaging analysis of specific mRNA expression based on the FRET-based DNA nano-tweezers technique. **H. Funabashi***, H. Shigeto, K. Nakatsuka, A. Kuroda
- 1080.** Development of rapid reciprocal-flow polymerase chain reaction system for quantitative analysis. **S. Furutani**, N. Naruishi, Y. Hagibara, H. Nagai*
- 1081.** Titin-based fluorescent tension sensors reveal the mechanochemistry of focal adhesions. **K. Galior***, Y. Liu, K. Yehl, K. salaita
- 1082.** Preparation of ruthenium complexes bearing a coumarin unit enables intracellular oxygen imaging. **D. Hara**, A. Son, K. Tanabe*, T. Kondo*

- 1083.** Raman imaging of ex vivo bone formation during osteoblast differentiation. **A. Hashimoto***, L. Chiu, C. Morimoto, K. Fujita, M. Takedachi, Y. Yamaguchi*, S. Kawata, S. Murakami, E. Tamiya*
- 1084.** Detection of circulating tumor cells in peripheral blood of lung cancer patients by use of a cell microarray chip. **Y. Hashimoto**, S. Yamamura, Y. Aoki, T. Hase, M. Kondo, Y. Hasegawa, Y. Baba, M. Kataoka*
- 1085.** Neuronal growth control using SAM modified nanopolymers as scaffolds. **N. Kasai***, A. Watanabe, R. Filip, A. Tanaka, T. Goto, Y. Kashimura, J. Brown, D. Sharp, S. Tsukada, J.F. Ryan, K. Sumitomo, H. Nakashima
- 1086.** Analysis of molecular mechanisms underlying ultraviolet-C induced circadian clock synchronization using luciferase probes. **G. Kawamura***, M. Hattori, T. Tamaru, T. Ozawa
- 1087.** Peptide nucleic acid that conjugates with a cell-penetrating peptide via a disulfide bond for detecting a specific small RNA inside cells. **M. Kitamatsu***, T. Ohtsuki
- 1088.** Graphical user interface, DeCon, for “in silico decontamination” of whole genome amplified bacterial single-cells. **T. Maruyama**, T. Mori, K. Yamagishi, H. Takeyama
- 1089.** Oscillation-assisted controlled release of biomolecules for high-efficient delivery to living cells using silicon nanoneedle array. **D. Matsumoto**, Y. Kato, R. Kawamura, T. Kobayashi, F. Iwata, C. Nakamura*
- 1090.** Identification of the producers of bioactive compounds from marine sponge by using Raman microspectroscopy. **R. Miyaoka**, M. Hosokawa, M. Ando, T. Mori, H. Hamaguchi, J. Piel, H. Takeyama
- 1091.** Concentration and purification by magnetic separation of cell or DNA using biochip. **N. Nagatani**
- 1092.** Single cancer cell isolation on the microcavity array platform using photopolymerizable hydrogel. **R. Negishi**, S. Nakamura, T. Saeki, M. Hosokawa, T. Tanaka, T. Matsunaga, T. Yoshino*
- 1093.** Picoliter-sized droplets for low bias whole genome amplification of single cell genome. **Y. Nishikawa**, M. Hosokawa, H. Takeyama
- 1094.** Construction of high-throughput inhibitor screening system for frequently mutated proteins of influenza virus. **R. Nishioka***
- 1095.** Development of antibody production system using goldfish toward single-cell analysis. **N. Nukada***, E. Avsar-Ban, Y. Tamaru
- 1096.** Microfluidic parallel extraction of chromosomal DNA molecules from single cells. **T. Oda**, T. Suzuki, H. Takao, F. Shimokawa, K. Terao*
- 1097.** Mass spectrometry for discovery and validation of neuropeptide genes in single neurons. **E. Romanova**, J.V. Sweedler*
- 1098.** 2D array multi-ion image sensor to individually and comprehensively analyze active response of stimulated cell. **H. Sato**, F. Dasai, R. Kato, K. Sawada, T. Hattori*
- 1099.** Superfine electrostatic inkjetting of monodisperse sub-femtoliter droplets for ultrarapid single-molecule in vitro compartmentalization. **B. Sharma**, T. Shimoda, Y. Takamura*, M. Biyani*
- 1100.** mRNA analysis of living cells after capturing SICM topography of the living cell membrane. **H. Shiku***, Y. Nashimoto, Y. Zhou, H. Ito, Y. Takahashi, K. Ino, T. Matsue
- 1101.** Detection of vimentin using antibody-modified nanoneedles and AFM to eliminate undifferentiated IPS cells. **K. Shimizu***, R. Kawamura, T. Kobayashi, M. Iijima, S. Kuroda, F. Iwata, K. Fukazawa, K. Ishihara, C. Nakamura
- 1102.** Development of thin-film lead zirconium titanate actuator using solution process for highly integrated biochip. **R. Shimura***, P. Trong Tue*, Y. Tagashira, Y. Ukita, T. Shimoda, Y. Takamura*
- 1103.** 3D microchamber with reagent reservoir for the single-cell analysis. **H. Suzuki***, K. Mitsuno, M. Tsugane, T. Okano, K. Shiroguchi
- 1104.** Solid-phase synthesis of gold nanoantenna as a nano-scale fluorescent light source. **S. Suzuki***, M. Yokokawa, H. Suzuki
- 1105.** Acceleration of on-chip immunoassays assisted by centrifugal thermal convection. **T. Tadokoro**, M. Saito, M. Murahashi, E. Tamiya*
- 1106.** Development of a bench-top extra-cleanroom for single cell genomics. **H. Takahashi**, T. Satoh*, H. Kanahara*, Y. Kubota*, T. Suzuki*, T. Kobori*, Y. Okamura*
- 1107.** Improving the electrochemical Imaging sensitivity of SECM-SICM by using size controllable Pt electrodeposited carbon nanoelectrode. **Y. Takahashi***, S. Mustafa, Y. Matsumae, Y. Nashimoto, H. Iida, K. Ino, H. Shiku, T. Matsue
- 1108.** Rapid circulating tumor cell detection based on wide-field fluorescent imaging system using 2D photosensor. **K. Takai**, R. Negishi, T. Saeki, Y. Maeda, T. Tanaka, T. Matsunaga, T. Yoshino*
- 1109.** Development of pipette tip-type biosensor for automated bioluminescence detection of target genes in pathogens. **E. Takano***, N. Shimura, K. Ikebukuro, T. Takeuchi
- 1110.** Live cell imaging and membrane protein mapping with atomic force microscope. **M. Takenaka***, T. Kobayashi, Y. Miyachi, K. Inokuma, J. Ishii, T. Hasunuma, C. Ogino, A. Kondo
- 1111.** Development of fish biotechnology for recombinant proteins and their antibodies toward single cell biosensing. **Y. Tamaru***
- 1112.** Electrochemical luminescent imaging of immunological cells inducing defense reactions with integrated microelectrode chamber array. **E. Tamiya**
- 1113.** Development of the image cytometry method to analyze g-protein coupled receptor kinetics in the cell. **M. Tan**, S. Yamahira, S. Yamaguchi, M. Nakamura, T. Nagamune
- 1114.** Label-free viable cells separation technique using deterministic lateral displacement microfluidic device. **N. Tottori**, J. Park, Y. Yanagida, T. Hatsuzawa
- 1115.** Solution-processed active matrix thin-film transistor for highly integrated biochip. **P. Trong Tue***, S. Inoue, T. Shimoda, Y. Takamura*
- 1116.** Development of a microfluidic chip for exosome study in single-cell analysis of exosome level. **K. Tsutsui**, W. Aoki, E. Wilfred, A. Hashimoto, M. Saito, E. Tamiya
- 1117.** Design of chemiluminescence system by combination of vinylphenols and naphthalene endoperoxide. **Y. Umehara**, K. Tanabe*, T. Kondo*
- 1118.** Extraction of the cytoplasm from single cell using planar patch clamp arrangement. **H. Uno**, Z. Wang, S. Ishigaki, T. Ishizuka, Y. Takamura, T. Urisu
- 1119.** Single cell genomic analysis of coral-associated uncultivable bacteria. **K. Yamagishi**, T. Mori, T. Maruyama, M. Ito, H. Takeyama
- 1120.** Collagen surfaces modified with photocleavable polyethylene glycol-lipid for versatile single-cell array available for both non-adherent and adherent cells. **S. Yamahira**, S. Yamaguchi*, M. Kawahara, T. Nagamune*
- 1121.** Development of on-site fluorescent measurement chip using photonic crystal. **Y. Yanagida***, Y. Imai, J. Park, T. Endo, T. Hatsuzawa
- 1122.** Development of cell microarray chip for rapid and high sensitive malaria diagnosis. **S. YATSUSHIRO**, S. Yamamura, M. SAKURAI, K. Abe, T. MITA, T. HORII, M. Kataoka
- 1123.** Rapid and selective detection of cysteine in living cells using a luciferin-inspired fluorogenic probe. **D. Ye***, M. Zheng, Y. Zhang

* Principle Author

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<http://pacifichem.org/onlineprogram>

- 10:10 – 1137.** ALS and FTLD-related protein aggregation induced by amyloidogenic peptides. **J. Huang***
- 10:40 – 1138.** Studies of protein misfolding diseases: Misfolding mechanism of prion protein and peptide therapy Alzheimer's disease. **R.P. Chen***, Y. Chiang, C. Yang

Sheraton Waikiki
Molokai

Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10)

Organized by: S. Silverman, Z. Huang, Y. Li, Y. Lu, H. Suga
Presiding: Z. Huang

- 8:00 – 1139.** RNA-catalyzed synthesis of RNA enzymes. **G. Joyce***, D. Horning, J. Szczepanski
- 8:25 – 1140.** DNA as a catalyst for biochemically relevant reactions in vitro and in vivo. **S.K. Silverman***
- 8:50 – 1141.** Small-molecule detection and enantiopurity measurement using DNA-based sensors. **J. Heemstra***
- 9:15 – 1142.** DNA-based asymmetric catalysis: Novel reactivity and DNA-induced rate acceleration. A. García Fernández, A. Draksharapu, A. Ríos Martínez, R.P. Megen, G. Roelfes*

9:40 Break

- 9:55 – 1143.** Genomic aptamers and ribozymes: From discovery to biological functions. **A. Luptak**

- 10:20 – 1144.** Deoxyribosensors: the de novo creation of chip-based electronic sensors made entirely out of DNA, for sensitive detection of disease biomarkers. **D. Sen***, J. Thomas, Y. Huang, H. Yu
- 10:45 – 1145.** Nearly two-decade pursuit of sequence specific RNase A mimics: Mission accomplished. **Y. Wang**, E. Liu, C.H. Lam, D. Perrin*
- 11:05 – 1146.** Genome-wide profiling of RNA folding in vivo. **P.C. Bevilacqua***

Sheraton Waikiki
Kauai

Biosynthesis of Natural Products (#27)

Organized by: I. Abe, B. Moore, D. Ro
Presiding: D. Ro

- 8:00 – 1147.** Enzyme-catalyzed [4 + 2]-cyclodaddition required for macrocyclization of spirotetrone-containing polyketides. **T. Kuzuyama***
- 8:30 – 1148.** Biosynthetic engineering to access altered thioether scaffolds. **W.L. Kelly**

- 8:50 – 1149.** From amide forming enzymes to discovery and engineering of bioactive molecules. **B. Li***, Z. Dunn, E. O'Neill, W. Wever
- 9:10 – 1150.** Hybrid RiPP pathways to create new bioactive scaffolds. **E.W. Schmidt**

- 9:40 – 1151.** In vitro biosynthetic system for peptides with diverse backbone heterocycles toward development of pseudonatural products. **Y. Goto***, Y. Kato, S. Tsumoda, Z. Suga
- 10:00 – 1152.** Reinventing natural product discovery. **D.A. Mitchell***

- 10:20 – 1153.** Peptide synthesis cooperatively achieved by peptide ligase and ribosomes. **T. Dairi**
- 10:50 – 1154.** Mechanistic studies on oxidative enzymes involved in the biosynthesis of peptidyl nucleoside antibiotics. **S.G. Van Lanen***, A. Goswami

- 11:10 – 1155.** Biosynthesis of streptothricin and its related antibiotics. **Y. Hamano***
- 11:30 – 1156.** How does one enzyme make and break 32 chemical bonds?. **W.A. van der Donk**

Sheraton Waikiki
Ewa

Homeostasis of Transition Metal Ions in Biological Systems (#47)

Organized by: S. Aono, D. Giedroc, J. Roe
Presiding: S. Aono, D.P. Giedroc

- 8:00 – 1157.** Spatio-temporal fluorescence analysis at the single cell level reveals zinc fluxes controlling the mammalian cell cycle. **T.V. O'Halloran**

- 8:30 – 1158.** Iron homeostasis in Saccharomyces cerevisiae. **P.A. Lindahl***, M.J. Moore, J.D. Wofford, S.P. McCormick

- 9:00 – 1159.** Organoferrorous agents for spatiotemporal disruption of iron homeostasis in cells. **J.M. O'Connor***, M.C. Aubrey, M. Proetto, C. Hoong

- 9:15 – 1160.** Iron-sulfur cluster assembly in bacteria. **D.R. Dean***

- 9:45 – 1161.** Cross-talk in metal homeostasis: Involvement of zinc in Fe-S cluster biogenesis in Bacillus subtilis. **P.C. Dos Santos***

- 10:15 – 1162.** Iron mobilization for metallo-cofactor biogenesis: Not all iron pools are equal. **F. Outten***, N. Bolaji

- 10:45 – 1163.** Iron-sparing response and iron uptake by Staphylococcus aureus. S.A. Loutet, M.J. Kobylarz, J.C. Grigg, M. Ikehata, **M.E. Murphy***

- 11:15 – 1164.** Unusual oxygenation mechanism of MuHdA, a heme degrading enzyme from *Mycobacterium tuberculosis*. **T. Matsui**, S. Nambu, S. Takahashi, H. Fujii, M. Ikeda-Saito

Sheraton Waikiki
Kahuku

Life at Small Copy Numbers (#137)

Organized by: S. Yoshimura, J. Xiao, P. Chen

Presiding: T. Nagai

- 8:00 – 1165.** Prospect of minority biology. **T. Nagai***

- 8:30 – 1166.** Bacterial hunger games: How bacteria ensure smooth gene expression during starvation. **M. Kim***

- 9:00 – 1167.** Gene expression in the low copy number limit. **R. Phillips***

9:30 break

- 9:40 – 1168.** Application of photoactive yellow protein as a photoresponsive module for controlling enzymatic activity. **M. Uri***, Y. Arai, M. Murakami, Y. Araki, T. Wada, H. Takahashi, K. Kirinba
- 10:00 – 1169.** Probing single-molecule mRNA and protein expression dynamics in *Saccharomyces cerevisiae*. **Y. Taniguchi***

10:20 break

- 10:30 – 1170.** Reaction networks with small copy numbers of molecules: Fluctuations and beyond. **Y. Togashi***

- 11:00 – 1171.** Noises and dynamics in cells: The fluctuation-dissipation theorem and the burst gene production model. **C. Hsu***, C. Yan

Hawaii Convention Center
Halls I, II, III

Biomolecular Structure and Dynamics: Recent Advances in NMR (#181)

Organized by: M. Tsai, A. Gronenborn, M. Ikura, W. Lee, G. Otting, I. Shimada

Poster Session

10:00 – 12:00

- 1172.** Solution structure of PKZ from Carassius auratus and its interaction with Z-DNA. **A. Lee**, J. Lee, J. Lee*

- 1173.** NMR study of various type III anti-freeze proteins explains their antifreezing activities. **s. Choi**, J. Lee, Y. Choi, J. Lee*

- 1174.** Structure and molecular mechanism of the microtubule severing enzyme using NMR. **N. Iwaya***, S. Noda, N. Goda, T. Tenno, H. Hiroaki

- 1175.** Triphosphate reorientation is a checkpoint in the fidelity mechanism of viral RNA-dependent RNA polymerase. X. Liu, X. Yang, D.M. Musser, **A.K. Boehr**, D.D. Boehr*

Royal Hawaiian
Regency I

Bioorganic Reaction Mechanisms (#224)

Organized by: J. Richard, M. Tanner, C. Easton

Presiding: J.W. Keillor

- 8:00 – 1176.** Novel enzymatic reaction mechanism found in biosynthesis of natural products. **H. Okawa***, A. Minami

- 8:30 – 1177.** Mechanism of enzyme-catalyzed retro-aldoxidations in *Mycobacterium tuberculosis*. **A.S. Murkin***, K.A. Manning, M.M. Moynihan

- 9:00 – 1178.** Regulation of human peptide hormone levels. **C.J. Easton***

- 9:30 – 1179.** Twisting tails and curious channels - the phosphoribosyltransferases. **E. Parker**, G. Mittelstaedt, T.V. Cookson

- 10:05 – 1180.** Transglutaminase conformation and function. **J.W. Keillor***, C. Clougherty, I. Roy

- 10:40 – 1181.** Multifunctional oxygenases in the biosynthesis of fungal meroterpenoids. **I. Abe***

- 11:10 – 1182.** Reaction mechanisms of radical SAM enzymes involved in the biosynthesis of aminoglycoside antibiotics. **F. Kudo***, S. Hoshi, T. Eguchi

Royal Hawaiian
Regency III

Function, Chemistry, and Signaling of Glycolipids and Phospholipids (#273)

Organized by: C. Cairo, M. Best, W. Cheng

Presiding: w. cheng

8:00 Opening remarks

- 8:05 – 1183.** Chemical approaches to the discovery and characterization of protein-membrane binding interactions using synthetic lipid probes. **M. Best***, M. Rowland, S. Eni Eni, S. Mattern-Schain

- 8:45 – 1184.** Probing intracellular signalling with inositol polyphosphates. **A.B. Holmes***, A.W. Burgess, B. Catimel, M.A. Gregory, M. Yin

- 9:25 – 1185.** Isotope-labeled phospholipids for examining domain-specific order profiles and compositional distribution by solid state NMR. **M. Murata***, T. Yasuda, J. Cui, M. Kinoshita, S. Matsuoka, N. Matsumori

10:05 Break

- 10:20 – 1186.** Diverse synthesis of glycophospholipids and their use in a study of bacterial cell wall assembly. **w. cheng***

- 11:00 – 1187.** Synthesis and evaluation of potential vaccines against Lyme disease based on the glycolipid BbGL1. **B.S. Huchenski, M. Hagar, S. Lee, T. Grindley***

- 11:20 – 1188.** Synthesis and biological studies of GPI anchors and GPI-anchored proteins. **Z. Guo**

Sheraton Waikiki
Honolulu

Chemistry and Applications of Retinal Proteins: From Microbes to Humans (#395)

Organized by: L. Brown, H. Kandori, M. Olivucci

Presiding: M. Olivucci

8:00 Introduction

- 8:05 – 1189.** Human infrared vision triggered by two-photon chromophore isomerization. **K. Palczewski***

- 8:35 – 1190.** Rhodopsin conformational dynamics in health and disease.

- O.P. Ernst***, L.N. Caro, N. Van Eps, T. Morizumi

- 9:05 – 1191.** Role of water and membrane lipids in rhodopsin activation. U. Chawla, S.M. Perera, B. Mertz, A.V. Struts, H. Liang, M.C. Pitman, **M.F. Brown***

- 9:20 – 1192.** Mechanism of rhodopsin activation by light-induced retinal isomerization. N. Kimata, M. Sheves, P. Reeves, **S.O. Smith***

- 9:50 – 1193.** Activation pathway of human rhodopsin in comparison to bovine rhodopsin. **F. Bartl***, R. Kazmin, S. Patrick, P. Hildebrand, E. Ritter

10:05 Break

- 10:15 – 1194.** Structural changes of squid rhodopsin during the thermal relaxation process in the P62 crystal. **M. Murakami*, T. Kouyama**

- 10:30 – 1195.** Thermal isomerization of chromophore in rod and cone visual pigments. **Y. Shichida**

- 11:00 – 1196.** Studies of spectral tuning and thermal decay of retinal photoreceptors. **V. Batista***

- 11:30 – 1197.** Role of rhodopsin's unusual kinetics of thermal reactions in dim-light vision. Y. Guo, S. Sekharan, V. Batista, J. Tully, **E. Yan***

Saturday Afternoon

Sheraton Waikiki
Kohala/Kona

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly, A. Smith, H. Suga, V. Nanda, J. Huang, K. Kudo, R. Cheng, P. Lyu

Presiding: R. Cheng

- 13:00 – 1198.** Structures, syntheses, and functions of antimicrobial peptides from gram positive bacteria. **J.C. Vederas**

- 13:30 – 1199.** Effect of membrane curvature on membrane translocation of arginine-rich peptides. **S. Futaki**

- 14:00 – 1200.** De novo-designed cationic foldamers from an unnatural δ -amino acid possess remarkable permeability to HeLa and primary neuronal cells. I. Monreal, E. Contreras, E. Paragas, G. Wayman, H. Aguilar, **J.P. Saludes***

- 14:20 – 1201.** Building protein mimics with robust cellular delivery activity. **G. Tew**

- 14:50 – 1202.** Effect of arginine modifications on structure and function. **R. Cheng**

- 15:20 – 1203.** Peptide nanostructures as molecular transporters of therapeutic agents. **K. Parang**, A. Nasrolahi Shirazi, R.K. Tiwari

- 15:40 – 1204.** Enzyme-mediated assembly of biomolecules on a designer scaffold based on self-assembled peptides. **R. Wakabayashi***, A. Suehiro, M. Goto, N. Kamiya*

- 16:00 – 1205.** Synthesis of protein-based biomaterials by genetically encoded Spy-Cap-SpyCatcher chemistry. **Y. Lu**, K. Minamihata, T. Nagamune

- 16:20 – 1206.** Racemic hydrogels from self-assembling enantiomeric peptides: Predictions from Linus Pauling. **J.P. Schneider**

Sheraton Waikiki
Molokai

Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10)

Organized by: S. Silverman, Z. Huang, Y. Li, Y. Lu, H. Suga

Presiding: Y. Lu

- 13:00 – 1207.** Biomarker discovery using DNA aptamers. **W. Tan**

* Principle Author

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<http://pacificchem.org/onlineprogram>

13:25 – 1208. Structure and metal ion binding properties of the mammalian CPEB3 ribozyme. **R.K. Sigel***

13:50 – 1209. RNA aptamer-conjugated liposomes as an efficient anticancer drug delivery vehicle targeting cancer cells *in vivo*. **D. Kim***, H. Park

14:10 – 1210. Targeting polymorphic DNA and their applications in disease diagnosis and treatment. **J. Wang, W. Li, P. Shi, Z. Zhang, J. Ren, X. Qu***

14:35 Break

14:50 – 1211. Developing DNA-based sensors for small molecule pollutant detection. **D.A. Baum***

15:15 – 1212. Turning the action of ligand-responsive functional DNAs into long-chain DNA amplicons via rolling circle amplification. **Y. Li**

15:40 – 1213. Development of various types of protein adaptors to locate a single molecule of functional protein on molecular switchboard. **T.A. Ngo*, E. Nakata, H.T. Dinh, T.M. Nguyen, M. Saimura, T. Mori**

16:00 – 1214. Highly selective fluorogenic probes for accurate and sensitive quantitation of nucleic acids. **J.A. Dallwig*, N. Ahnert, T. Huang, K. Gee, D. Gale, A. Dix**

16:25 – 1215. Optical control of oligonucleotide function in cells and animals. **A. Deiters**

Sheraton Waikiki
Kauai

Biosynthesis of Natural Products (#27)

Organized by: I. Abe, B. Moore, D. Ro
Presiding: T. Mahmud

13:00 – 1216. Genetic strategies for molecular diversity. **J. Clardy*, C. Currie, A. Ruzzini, E. Van Arnam, C. Sit**

13:30 – 1217. Combined-culture: The new method for secondary metabolism activation in actinomycetes. **H. Onaka***

13:50 – 1218. Chemical discovery in the microbial world. **E.P. Balskus***

14:10 – 1219. Insights from a global view of secondary metabolism: Small molecules from the human microbiota.

M. Fischbach

14:40 – 1220. Probing the biosynthetic capabilities of a marine *Nocardiosis* sp. **A.L. Lane**

15:00 – 1221. Uncovering new molecules and biosynthetic pathways from marine bacteria. **A. Ross***

15:20 – 1222. Culture independent approaches for the discovery of new bacterial metabolites. **S. Brady**

15:50 – 1223. Development of the heterologous expression technology applicable for huge biosynthetic gene clusters.

K. Shin-ya*

16:10 – 1224. Natural products library initiative (NPL) at TSRI – reflections and prospective. **B. Shen***

16:40 – 1225. Novel alkaloidal phytoalexins and their biosynthetic pathways. **M.c. Pedras*, Q. To**

Sheraton Waikiki
Ewa

Homeostasis of Transition Metal Ions in Biological Systems (#47)

Organized by: S. Aono, D. Giedroc, J. Roe
Presiding: K. Ishimori, J. Roe

13:00 – 1226. Mechanistic insights into iron regulation in yeast. **C.E. Outten***

13:15 – 1227. Structural basis of the bacterial heme transporter. **H. Sugimoto***

13:45 – 1228. From the cytoplasm to the periplasm and beyond, passing the Cu⁺ along. **J.M. Arguello***

14:15 – 1229. Metal trafficking in cells through a cellular structural biology approach. **L. Banci***

14:45 – 1230. Determinants of nickel site selectivity and sensitivity in transport, trafficking, and regulation. **P. Chivers***

15:15 – 1231. On the pathways adopted by metallothionein in binding, sequestering, and finally donating zinc to zinc-dependent enzymes. **M. Stillman***

15:45 – 1232. Is copper involved in the function of the amyloid precursor protein?. **A.G. Wedd*, Z. Xiao, T. Young**

16:15 – 1233. Lost in metallation: The disaster on a protein structure leading to neurodegeneration. **Y. Furukawa*, I. Anzai, K. Nagasawa, S. Akiyama, M. Imai, K. Ishimori**

16:30 – 1234. Is the mycobacterial protein nanocage involved in oxidative stress response?. **H. Contreras, S. Dixon, C. Goulding***

Sheraton Waikiki
Kahuku

Life at Small Copy Numbers (#137)

Organized by: S. Yoshimura, J. Xiao, P. Chen
Presiding: H.R. Ueda

13:00 opening remark

13:05 – 1235. Toward organisms-level systems biology. **H.R. Ueda**

13:35 – 1236. Cell size control and homeostasis of individual cells. **S. Jun***

14:05 – 1237. How is a long strand of genomic DNA organized in the cell?. **K. Maeshima**

14:25 break

14:35 – 1238. Harnessing ‘noise’ for cell-fate manipulation and therapy. **L. Weinberger***

15:05 – 1239. Adiabatic and non-adiabatic nonequilibrium stochastic dynamics of single regulating genes. **J. Wang***

15:35 – 1240. Structure and dynamics of protein complex in macromolecular crowding. **S. Yoshimura, H.A. Konishi, S. Asai, M. Kumeta**

15:55 break

16:05 – 1241. Combinatorial gene regulation by pulse timing modulation. **Y. Lin**

16:35 – 1242. Distribution of genome-size DNA in the dividing model cell membrane. **H. Suzuki***

16:55 closing remark

Royal Hawaiian
Regency I

Bioorganic Reaction Mechanisms (#224)

Organized by: J. Richard, M. Tanner, C. Easton
Presiding: J. Pelletier

13:00 – 1243. Discovery, evolution, and mechanism of a new family of nonheme iron halogenases that act on free substrates Independent of carrier protein. **X. Liu**

13:20 – 1244. Extended network of proximal and distal hydrogen bonds delivers RhoA catalyzed GTP hydrolysis via a strain-free transition state. **N. Richards, R. Molt, Y. Jin, E. Pellegrini, M. Bowler, J. Walther, M. Blackburn**

13:45 – 1245. Energetics of the proton-transfer mechanism in aspartate aminotransferase. **H. Hayashi*, T. Murakawa, M. Shoji, Y. Shigeta**

14:20 – 1246. Design and optimization of artificial enzymes: Nearer to nature. **D. Hilvert***

15:00 – 1247. Discovery and improvement of novel glycosidases through metagenomics and directed evolution. **S.G. Withers, S. Hallam, z. Armstrong, K. Mewis, F. Liu, T. Duo**

15:40 – 1248. Engineering biocatalysts: Exploring and exploiting flavoenzymes. **S. Lutz**

16:20 – 1249. Does engineering functional enzymes require preserving protein dynamics?. **J. Pelletier*, S. Gobael, C. Clouthier, J. Park, D. Gagné, A. Berghuis, N. Doucet**

Royal Hawaiian
Regency III

Function, Chemistry, and Signaling of Glycolipids and Phospholipids (#273)

Organized by: C. Cairo, M. Best, W. Cheng
Presiding: C. Cairo

13:00 Opening remarks

13:05 – 1250. Investigation of the assembly and budding of *filoviruses* from the host cell plasma membrane. **R.V. Stahelin***

13:45 – 1251. Lipidomic profile of gut commensal bacteroidales and identification of immunomodulatory glycosphingolipids. **S.F. Oh*, W. Zheng, H. Song, h. kim, S. Park, D.L. Kasper**

14:05 – 1252. Detection of lipid-linked peptidoglycan precursors by exploiting an unexpected transpeptidase reaction. **Y. Qiao, M. Lebar, K. Schirmer, K. Schaefer, H. Tsukamoto, D. Kahne*, S. Walker***

14:25 – 1253. Fluorescence- and Raman-based spectroscopies for cell membrane measurements. **E.A. Smith, A. Syed, Q. Zhu, C. Wijesooriya**

15:05 Break

15:20 – 1254. Ganglioside probes for exploring functional molecular complexes in the cell membrane. **H. Ando***

16:00 – 1255. Cationic glycolipids as potent antimutant agents. **M. Ogunsina, T. Idowu, P. Samadder, G. Arthur, F. Schweizer***

16:20 – 1256. Monitoring enzymatic cleavage of phospholipids in symmetric lipid bilayers with vibrational sum frequency generation. **J. Gibbs-Davis**

Saturday Evening

Sheraton Waikiki
Kohala/Kona

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly, A. Smith, H. Suga, V. Nanda, J. Huang, K. Kudo, R. Cheng, P. Lyu
Presiding: K. Kudo

19:00 – 1257. Orthogonal protection strategies of Schollkopf's *bis*-lactim ether for the synthesis of non-proteinogenic dipeptides and α-amino acids. **M. Hutchby*, S.D. Bull**

19:20 – 1258. Use of cyclic dipeptides as receptors and chiral catalysts. **C. Bérubé*, C. Bouchard, S. Cardinal, N. Voyer**

19:40 – 1259. Dual functionalization and glycosylation of native amino acids. **D. Skropeta, C.J. Cara**

20:00 – 1260. Lipid-modified peptides: New synthetic strategies, protecting groups, and combinatorial methods. **M. Distefano*, V. Diaz-Rodriguez, M. Mahmoodi**

20:20 – 1261. Covalent molecular recognition: Iminoborionate chemistry in water. **J. Gao***

20:40 – 1262. Different CMT disease-causing mutations promote the same neomorphic conformation of human GlyRS. **W. He**

Hawaii Convention Center
Halls I, II, III

Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10)

Organized by: S. Silverman, Z. Huang, Y. Li, Y. Lu, H. Suga
Presiding: S.K. Silverman

Poster Session

19:00 – 21:00

1263. Structural stability and metal ion selectivity of the *yybP*-*ykoy* riboswitch. **L. Cavallo*, M. Chawla, R. Credendino, R. Oliva**

1264. Functional and structural analyses of c-di-GMP responsive riboswitch. **S. Inuzuka, K. Nishimura, H. Kakizawa, H. Furuta, S. Matsumura, Y. Ikawa***

1265. Rational engineering of ribosomal shunt-modulating eukaryotic ON-riboswitches. **A. Ogawa***

1266. Construction and screening of the RNP library with catalytic functional group. **T. Tamura, K. Ariyama, S. Nakano, T. Morii**

1267. DNA-catalyzed conjugation of nucleic acids and tyrosine side chains. **C. Chu, S.K. Silverman***

1269. DNA catalysts with chemically modified nucleotides to hydrolyze amide bonds. **C. Zhou, S.K. Silverman***

1270. Selection of catalytic DNA with O-glycosidase activity. **C. Yeh, J. Chandrasekar, S.K. Silverman***

1271. DNA-catalyzed PEgylation of peptides and proteins. **P. Wang, S.K. Silverman***

1272. Selection and characterization of X-aptamers for small molecules. **P.K. Tsae, M.C. DeRosa***

1273. Dopamine-binding DNA aptamer therapeutics for the treatment of schizophrenia and addiction. **E.M. McConnell*, M.R. Holahan, M.C. DeRosa**

1274. Application of oligonucleotide-templated chemical reactions to DNA aptamers for the detection of circulating tumor cells using terahertz chemicalmicroscopy. **E.M. Hassan**

1276. Design and evaluation of the specific ligand for CTG repeat sequence. **J. MATSUMOTO, J. Li, K. NAKATANI***

1277. Small-molecule inhibitor of pre-miR-29 maturation. **A. Murata, T. Otabe, J. Zhang, K. NAKATANI***

1278. SPR-based in vitro selection of pre-miRNA loop mutant molecules that bind to the restrained naphthyridine dimer. **Y. Mori*, Y. Di, A. Sugai, A. Murata, K. NAKATANI**

1279. Analysis of binding of naphthyridine-azaquinolone derivatives to CAG repeats RNA. **A. Sakata, J. Li, H. He, A. Murata, C. Dohno, S. Obika, K. NAKATANI***

1280. Integrated biophysical approaches to determine structures of the steroid receptor activator lncRNA ribonucleoprotein complexes. **T.C. Leeper*, S. Bilinovich, C. Davis, J. Caporaso, D.L. Morris**

1281. Synthesis and properties of functional trinucleotide repeat-binding molecules to induce chemical transformation of trinucleotide repeats. **T. Yamada*, K. NAKATANI, A. Michikawa**

1282. Design of triple-forming RNA transcription factor. **M. Noda, T. Yamamoto, S. Hori, Y. Hari, S. Obika***

1283. Selection of modified DNA aptamers: Comparison of capillary electrophoresis and biolayer interferometry. **Y. Kasahara*, K. Hagiwara, M. Kuwahara, S. Obika**

1284. Development of high sensitivity aptamer based diagnostic kit for aminoglycoside antibiotics. **M. Yoon***

1285. Screening method to obtain aptamers binding different sites of the target molecule. **Y. Yamamoto, K. Abe, N. Savory, K. Ikebukuro***

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- 1286.** Investigation of the effects of G-quadruplex ligand (7OTD) on the expression of cell transcriptome. **T. Saito**, T. Yokoyama, K. Teramoto, W. Yoshida, K. Abe, K. Iida, K. Nagasawa, K. Ikebukuro*
- 1287.** Characterization of aptamer forming G-quadruplex structure and its binding to target molecules in hydrated ionic liquid. **T. Honda**, K. Abe, K. Fujita, H. Ohno, K. Ikebukuro*
- 1288.** Abridged pathway for modification of 2-thiouridine tRNA in *Bacillus subtilis*. **P.C. Dos Santos***, K. Black
- 1289.** Construction of metallo-DNA duplexes using 5-hydroxyuracil nucleobases as metal coordination sites. **K. Nishiyama**, Y. Takezawa, T. Mashima, M. Katahira, M. Shionoya
- 1290.** Artificial metallo-DNA three-way junction: Metal-mediated stabilization and structural induction. **Y. Takezawa**, S. Yoneda, J. Duprey, M. Shionoya*
- 1291.** DNA-binding studies of pyrrole-imidazole polyamides with anti-HPV activity. **M.J. Scuderi**, K.J. Koeller, T.G. Edwards, C. Fisher*, G. He, G.D. Harris, C.M. Dupureur, J.K. Bashkin*
- 1292.** Intrinsically fluorescent nucleoside analogs: Synthesis, properties, and applications. **R. Hudson***
- 1293.** Submolecular dissection reveals loop interaction is stronger than π - π stacking for G-quadruplex stability. **C. Ghimire**, S. Park, K. Nagasawa, H. Sugiyama, H. Mao*
- 1294.** Locating the uracil-5'-yl radical formed in DNA containing 5-bromouracil. **F. Hashiya***, H. Sugiyama
- 1295.** Design and photophysical properties of an environmentally sensitive fluorescent nucleoside, 3-deaza-2'-deoxyadenosine derivative: Distinguishing thymine by probing the DNA minor groove. **Y. Saito**, A. Suzuki
- 1296.** 7-deaza-8-azadenine and its 7-substituted derivatives: Structural and energetic impact on H-bonding potential with uracil in RNA molecules. **R. Oliva**, M. Chawla, R. Credendino, L. Cavallo
- 1297.** Base-ribose stacking in functional RNAs: Bioinformatics and quantum mechanics characterization. **R. Oliva**, M. Chawla, E. Chermak, J. Bujnicki, L. Cavallo
- 1298.** Screening method for RNA G-quadruplex stabilizers. **Y. Katsuda**, S. Sato, M. Uesugi*
- 1299.** Construction of homo- and hetero-oligomers of peryleneimide derivatives in a DNA duplex by using abasic sites as binding and reactive sites. **T. Takada***, K. Yamana
- 1300.** Synthesis and applications of new fluorescent deoxyribonucleoside analogs. **S. Yamamoto**, S. Park, H. Sugiyama*
- 1301.** Live-cell imaging of endogenous mRNAs with a small molecule. **S. Sato**, Y. Katsuda, M. Watanabe, M. Uesugi*
- 1302.** Development of environmentally sensitive fluorescent 8-aza-7-deazapurine nucleosides forming stable Watson-Crick base pairs. **A. Suzuki**, Y. Saito*
- 1303.** Water-soluble nucleotide analog with a flexible backbone and positive charges. **Y. Watanabe**, M. Kuwahara*
- 1304.** Regulation of translational activity of EGFP mRNA using photoresponsive α -haloaldehyde-conjugated ORNs. **Y. Nakata**, Y. Sugihara, A. Kobori, A. Yamayoshi, A. Murakami
- 1305.** Development of novel anti-HIV drugs that mimic functions of non-coding RNA. A. Yamayoshi*, K. Yoshimoto, K. Ishimoto, A. Kobori, A. Murakami, J. Ariyoshi
- 1306.** Introducing azaHx, a novel fluorescent, DNA sequence specific, minor groove, and GC recognition element: Expanding the scope of Hx-amide DNA sequence recognition. V. Satam, B. Babu, P. Patil, K. Olson, M. Savagian, M. Lee, A. Mepham, C. Bruce, S. Wang, D. Wilson, K. Kiakos, J. Hartley, M. Lee*
- 1307.** Efficient covalent capture of 8-nitroguanosine via a multiple hydrogen-bonded complex. **Y. Fuchi**, S. Sasaki
- 1308.** Dynamic and mutual chiral induction system between B-, Z-DNA and the chiral [5]helicene-spermine ligand. **K. Kawara**, S. Sasaki
- 1309.** Selective and cooperative binding of small molecular ligands to a GC repetitive site of DNA mediated by multiple competition with metal cations. **H. Murase**, S. Sasaki
- 1310.** Recognition and discrimination between 8-oxo-2'-deoxyguanosine and 2'-deoxyguanosine in DNA using the adenosine-1,3-diazaphenoxazine nucleoside derivatives. **Y. Taniguchi***, Y. Kikukawa, S. Sasaki
- 1311.** Stiylactose-modified 3-way junction DNA as an inhibitor of influenza hemagglutinin. **Y. Ebara**, M. Yamabe, D. Akamatsu, K. Kaihatsu, N. Kato
- 1312.** Novel inhibitors targeting microRNA: Peptide oligonucleotide conjugates for promotional releasing of microRNA from RISC. **J. Ariyoshi**, N. Eimori, R. Konishi, A. Kobori, A. Murakami, A. Yamayoshi
- 1313.** Development of oligonucleotides having a caged α -haloaldehyde group and their inhibitory effect on translational activity of EGFP mRNA. **Y. Sugihara**, Y. Nakata, A. Yamayoshi, A. Murakami, A. Kobori*
- 1314.** Analysis of alternative splicing by homogeneous fluorescence assay. **K. Nakajima**, A. Nishimura, A. Yamayoshi, A. Murakami, A. Kobori*
- 1315.** Photoresponsible cap for reversible regulation of translation. **S. Ogasawara***
- 1316.** Development of a novel fluorescence in situ hybridization method using photo-reactive oligonucleotide as a fluorescent probe. **K. Toyosato**, T. Sakamoto, S. Nakamura, K. Fujimoto*
- 1317.** 19F NMR-based analysis of the local sequence and structure of DNAs using fluorine-modified bisbenzimidazole derivative. **D. Hasegawa**, T. Sakamoto, K. Fujimoto*
- 1318.** Partial complementarity guided predictable and reliable synthesis of inter-strand crosslinked oligonucleotides. B. Yoo, N. Persky, R. Wang, F. Yannick, C. Martinez, N. Pavletich, O. Ouerelli*
- 1319.** Combining structure-switching aptamers with rolling circle amplification for biosensor development. **R.M. Bialy**, Y. Li, J.D. Brennan*
- 1320.** Aptamer immobilization on comb-branched DNA scaffolds for bioanalytical applications. **E.K. TeSelle**, D.A. Baum
- 1321.** Rational design of DNA-based sensing systems with precisely defined operational parameters. **I.V. Nesterova**
- 1322.** Rapid identification of RNA viruses by peptide nucleic acid chromatography. **K. Kaihatsu**, S. Sawada, K. Takagi, T. Hayashi, M. Okazaki, N. Kato
- 1323.** Photoligation-based quantitative technology for transcriptome analysis without reverse transcription. **M. Yokomori**, A. Suyama
- 1324.** Quantitative detection of a single base change in RNA with DNazyme and graphene oxide. **D. Kim***, C. Hong, A. Baek, D. Kim
- 1325.** Orthogonal assembly of RuBisCO and carbonic anhydrase on a DNA nanoscaffold. **H.T. Dinh**, E. Nakata, T.A. Ngo, H. Ashida, T. Morii
- 1326.** Specific detection of ATP by fluorescent ribonucleoprotein sensors. **S. Nakano**, T. Tamura, T. Morii*
- 1327.** Development of modular adaptors to covalently locate multiple enzymes on DNA nanoscaffold. **T.M. Nguyen***, E. Nakata, H.T. Dinh, T.A. Ngo, M. Sairuma, T. Morii
- 1328.** New approach to detection of target DNA or RNA by coloring PALSAR method. **R. Morinaka**, N. Kato, A. Ohno, H. Haraguchi, S. Futo
- 1329.** Detection of *Legionella* in hot spring water using the coloring PALSAR method. **H. Haraguchi**, R. Morinaka*, N. Kato, A. Ohno, S. Futo
- 1330.** Construction of an RNA device based on a splicing ribozyme for amplification of input-signals. **R. Kiyooka**, S. Matsumura, Y. Ikawa*
- 1331.** Programmable formation of catalytic 1D and 2D RNA nanostructures by assembling group I ribozymes. **S. Matsumura**, N. Uehara, D. Fujita, H. Furuta, Y. Ikawa*
- 1332.** Intracellular delivery of impermeable photosensitizer by DNA tetrahedron and its potential for photodynamic therapy. **D. Ahn***
- 1333.** Lipid-bilayer-assisted 2D self-assembly of DNA origami nanostructures. **Y. Suzuki**, M. Endo, H. Sugiyama
- 1334.** Single-molecule manipulation and visualization of multiple DNA structural changes in the DNA nanostructures using high-speed AFM. **M. Endo**, H. Sugiyama
- 1335.** DNA nanotechnology for controlling receptor signaling. **R. Ueki**, N. Kanda, A. Utsumi, S. Sando*
- 1336.** Construction of chromophore arrays using DNA. **M. Nakamura***, T. Takada, K. Yamana
- 1337.** Study of the dynamics of DNA nanotubes. **j. rahban***, A. Hariri, G. Cosa, H. Sleiman
- 1338.** Development of orientation-dependent FRET system for structural analyses of nucleic acids. **H. Kashida**, A. Kurihara, H. Asanuma*
- 1339.** Combination of histone deacetylase inhibitors and lipofection-mediated INF- β gene therapy. **R. Nishimura**, H. Aihara, M. Katsuragi, Y. Fukushima, S. Uesato, T. Sumiyoshi, Y. Nagaoka*
- Sheraton Waikiki
Kauai
- Biosynthesis of Natural Products (#27)**
- Organized by: I. Abe, B. Moore, D. Ro
Presiding: J.C. Vederas
- 19:00 – 1340. Unlocking the mystery of natural rubber (*cis*-1,4-polyisoprene) biosynthesis in lettuce. **D. Ro***, Y. Qu, C. Romit, M. Kwon, E. Kwon
- 19:20 – 1341. Direct protein structure and function in *planta*: Evolutionary and metabolic ramifications. **N.G. Lewis**, K. Kim, H.K. Senaratne, C.A. Smith, M. Daily, J.R. Cort, L.B. Davin
- 19:40 – 1342. Biosynthetic study of plant specialized products by means of genomics and metabolomics. **K. Saito***
- 20:10 – 1343. Mining the *Cannabis sativa* genome: Identification of *cannabichromenic acid synthase*. **J. Stout**, J. Page
- 20:30 – 1344. Discovery and assembly of pathways for medicinal monoterpenoid indole alkaloids in plants and microorganisms. **V. De Luca**
- Hawaii Convention Center
Halls I, II, III
- Homeostasis of Transition Metal Ions in Biological Systems (#47)**
- Organized by: S. Aono, D. Giedroc, J. Roe
- Poster Session
19:00 – 21:00
1345. Spectroscopic properties of heme-binding protein HupD responsible for heme acquisition in *Listeria monocytogenes*. Y. Okamoto, M. Ogura, T. Uchida, K. Ishimori, T. Hayashi, **S. Aono***
1346. Structural basis for heme acquisition in *Corynebacterium glutamicum*. **N. Muraki**, Y. Okamoto, C. Kitatsui, S. Aono
1347. Small-angle X-ray scattering analysis reveals the overall structure and signal transduction mechanism of a heme-based oxygen sensor protein, FixL. **A. Saeki**, T. Hikima, G.S. Wright, S.V. Antonyuk, S. Hasnain, M. Yamamoto, Y. Shirio, H. Sawai*
1348. Genetic response against removal of CO from the blood of mice by an iron(II)-porphyrin-cyclodextrin supramolecular complex. **S. Minegishi**, H. Kitagishi*, A. Yumura, S. Negi, Y. Sugiyura, K. Kano
- Hawaii Convention Center
Halls I, II, III
- Function, Chemistry, and Signaling of Glycolipids and Phospholipids (#273)**
- Organized by: C. Cairo, M. Best, W. Cheng
- Poster Session
19:00 – 21:00
1360. High levels of arachidonic and n-3 docosapentaenoic acid in the phospholipids of marine gastropod *Turbo cornutus*. **h. saito***
1361. Novel synthesis of deuterated phosphatidylinositol 4,5-bisphosphate. **A.M. Saunders**, H. Sangane, V. Flemington, S.J. Conway
1362. Ergosterol-glucosidase catabolism by ergosterol- β -glucosidase (Egh1) is associated with vacuole formation in *Saccharomyces cerevisiae*. **T. Watanabe**, M. Tani, Y. Ishibashi, N. Okino, M. Ito

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- 1363.** Theoretical interaction analysis between hemagglutinin of influenza A virus and sulfate. **Y. Fujita**, S. Okazaki, T. Takahashi, K. Ikeda, T. Suzuki, H. TOKIWA*
- 1364.** Development of detection system of amyloid β peptide from Alzheimer's disease using lipid membranes: A quartz crystal microbalance method. **T. Shimanouchi**, M. Iwamura, Y. Sano, Y. Kimura
- 1365.** In vivo clearance of secreted phospholipase A2 from extracellular medium by the M-type receptor. **H.N. Ewing***, G. Naika, F. Ghomashchi, M.H. Gelb
- 1366.** Development of a new approach to prepare structurally diverse peptidoglycan intermediates: Synthesis and functional study of N-substituted lipid II analogs. **C. Guo**, C. Lin*, w. cheng*
- 1367.** S-linked sialyloligosaccharides bearing lipid for influenza virus inhibition. **P. Liang**, Y. Lee

Hawaii Convention Center
Halls I, II, III

Chemistry and Applications of Retinal Proteins: From Microbes to Humans (#395)

Organized by: L. Brown, H. Kandori, M. Olivucci
Presiding: L. Brown

Poster Session
19:00 – 21:00

- 1368.** Mechanism of ion-conducting pore formation and gating in Channelrhodopsin-2. **F. Bartl***
- 1369.** Novel group of eubacterial proton pumps with the unique proton-donating complex. **L. Brown***, A. Harris, M. Ljumovic, S. Ito, K. Inoue, H. Kandori, A. Bondar
- 1370.** Reversible hydration-volume fluctuations in rhodopsin activation: Scattering and NMR methods confirm molecular dynamics predictions. X. Xu, S.M. Perera, U. Chawla, U. Shrestha, T.R. Molugu, A.V. Struts, D. Bhowmik, J. Feng, N. Nesnas, B. Mertz, M.C. Pitman, X. Chu, **M.F. Brown***
- 1371.** Light-driven sodium ion pumping activity is controlled by positive and negative charged residues in new type of microbial rhodopsin. **A. Choi***, S. Kim, K. Lee, S. Kim, S. Bae, K. Koo, H. Shin, K. Jung

- 1372.** Arrestin splice-variant p44 delays retinal release from photoactivated rhodopsin via meta III. **C.E. Eckert***, D. Chatterjee, C. Slavov, K. Saxena, C. Sanders, V.V. Gurevich, J. Wachtveitl, H. Schwalbe

- 1373.** Comparison of bovine and human rhodopsin photoactivation kinetics. **C. Funatogawa**, I. Szundi, D.S. Kliger*, J. Lewis

- 1374.** FTIR spectroscopy of animal and microbial rhodopsins. **H. Kandori**

- 1375.** Photochemical characterization of flavobacterial rhodopsin: The importance of the helix E region for heat stability. **S. Kim***, S. Han*, J. Cho, K. Lee, K. Shin, G. Lee, K. Jung

- 1376.** Function and photochemical properties of actinohrhodopsins. **S. Kim***, K. Jung, J. Park

- 1377.** Electronic progression during the photoisomerization of microbial and animal light-sensing rhodopsins. **M. Olivucci***, H. Luk, F. Melaccio, S. Rinaldi, S. Gozem

- 1378.** Tracking folding events during cell-free expression of bacteriorhodopsin into nanodiscs by SEIRAS. **R. Schlesinger***, K. Ataka

- 1379.** Inversion of sequence and direction of the proton transfer in proteorhodopsin at high pH. **J. Tamogami***, T. Kikukawa, T. Nara, M. Demura, E. Muneyuki, N. Kamo

Sunday Morning

Sheraton Waikiki
Kohala/Kona

Advances in Peptide and Protein Chemistry (#6)

Organized by: W. Lubell, J. Kelly, A. Smith, H. Suga, V. Nanda, J. Huang, K. Kudo, R. Cheng, P. Lyu
Presiding: P. Lyu

- 8:00 – 1380.** Protein-based hybrid catalysts for hydrogen production. **G. Ghirlanda***

- 8:30 – 1381.** Dressed up artificial viral capsids self-assembled from β -annulus peptides. **K. MATSUURA***, T. Honjo, T. Iwasaki

- 8:50 – 1382.** Construction of a bispecific antibody via protein trans-splicing. Y. Shibuya, R. Asano, H. Nakazawa, M. Umetsu, K. makabe*

- 9:10 – 1383.** Chemical synthesis of homogeneous glycoprotein and an insight into the relationship between glycosylation pattern and biological activity. **Y. Kajihara**

- 9:30 – 1384.** RE3Volutionary computational design of symmetric proteins. **A.R. Voet**

- 9:50 – 1385.** Single mutations in a non-enzymatic protein give rise to various catalytic activities. Y. Moroz, T. Dunston, O. Moroz, O. Makhlynets, Y. Wu, P. Gosavi, J. Yoon, N. van Nuland, I. Korendovych*

- 10:10 – 1386.** Site-specific protein PEGylation through incorporation of aromatic amine-containing non-natural amino acid. **T. Watanabe**, R. Shiba, T. Hohsaka*

- 10:30 – 1387.** Organometallic palladium complexes as chemoselective bioconjugation reagents. **E.V. Vinogradova**, C. Zhang, A. Spokony, B. Pentelute, S. Buchwald, B.F. Cravatt

- 10:50 – 1388.** Posttranslationally modified tau proteins accessed by a novel purification tag. **O. Reimann**, C. Smet-Nocca, C.P. Hackenberger*

- 11:10 – 1389.** Effect of chemical modifications of amino acids as point mutations in protein function. S. Sakurai, A. Tsuneshige*

- 11:30 – 1390.** ME47, a minimal protein designed to target the Myc/Max:E-box DNA network, decreases cancer cell growth. **J. Shin***

Sheraton Waikiki
Molokai

Functional Nucleic Acids: Chemistry, Biology, and Materials Applications (#10)

Organized by: S. Silverman, Z. Huang, Y. Li, Y. Lu, H. Suga
Presiding: S.K. Silverman

- 8:00 – 1391.** Crystal structure of an RNA mimic of GFP reveals a G-quadruplex core. **A.R. Ferre-D'Amare***

- 8:25 – 1392.** Development of aptasensors for the detection of organic compounds contaminated in foods. **Y. Morita**, Y. Tomita, D. Fujiwara, H. Suga*

- 8:50 – 1393.** Responsive aptamer-based materials and nanoswitches. **M.C. DeRosa***

- 9:10 – 1394.** Conserved ligand-responsive RNA switches regulating viral translation. **T. Hermann***, M.A. Boerneke

- 9:35 Break**
9:50 – 1395. Platinum biomolecule target analysis using click chemistry. J.D. White, A. Moghaddam, R. Cunningham, K. Plakos, E. Reister, M.M. Haley, V. DeRose*

- 10:15 – 1396.** DNA nanowire field-effect transistor. **K. Yamana***, T. Takada, N. Matsu

- 10:35 – 1397.** Artificially expanded genetic information systems (AEGIS) for creating receptors, ligands, and catalysts on demand. **S. Benner***, R.W. Shaw, M. Matsura

- 11:00 – 1398.** Creation of high affinity DNA aptamers using a genetic alphabet expansion toward diagnostic and therapeutic applications. **I. Hirao***

- 11:25 – 1399.** Semi-synthetic organism with an expanded genetic alphabet. **F. Romesberg**

- 11:50 Closing remarks**

Sheraton Waikiki
Kauai

Biosynthesis of Natural Products (#27)

Organized by: I. Abe, B. Moore, D. Ro
Presiding: I. Abe

- 8:00 – 1400.** Novel terpenes generated by awakening of genes encoding bacterial terpene synthase. **H. Ikeda**

- 8:30 – 1401.** Tools to investigate carrier protein biosynthesis. **M. Burkart**

- 9:00 – 1402.** Biosynthesis of a diazo-containing natural product from *Streptomyces*. **Y. Katsuyama**, Y. Ohnishi

- 9:20 – 1403.** Azinomycin biosynthesis: probing the mechanism of azacyclic biosynthesis. **C. Watanabe***, K. Nepal, S. Mori, D. Simkhada, V. Sharma, G. Kelly, D. Delgado

- 9:40 – 1404.** Posttranslational isoprenylation of tryptophan. **M. Okada**

- 9:55 – 1405.** Lincomycin biosynthesis: a tale of two small-molecule thiols. Q. Zhao, M. Wang, W. Liu*

- 10:25 – 1406.** Mechanistic studies on a new menaquinone biosynthetic pathway. **T.P. Begley***

- 10:55 – 1407.** Biosynthesis and tailoring of marine microbial siderophores. **A. Butler***

- 11:15 – 1408.** Characterization of two novel plant type III polyketide synthases obtained from medicinal plant *Evodia rutaecarpa*. **H. Morita***, T. Kodama, H. Noguchi, I. Abe

- 11:30 – 1409.** Mechanism-based self alkylation in sesquiterpene synthases. **J.P. Noel***, R.D. Kersten

Sheraton Waikiki
Ewa

Homeostasis of Transition Metal Ions in Biological Systems (#47)

Organized by: S. Aono, D. Giedroc, J. Roe
Presiding: P. Chivers, P.A. Lindahl

- 8:00 – 1410.** Molecular mechanisms of heme homeostasis in Gram-positive bacteria. **S. Aono***

- 8:30 – 1411.** Specific heme binding in iron regulatory proteins and its functional significance. **K. Ishimori**

- 9:00 – 1412.** CCHC 'zinc finger' proteins that regulate RNA processing: Metal ion switching and RNA recognition. **S. Michel***

- 9:30 – 1413.** Bacterial riboswitches cooperatively bind Ni(II) or Co(II) and control expression of heavy metal transporters. **W. Winkler**

- 10:00 – 1414.** Regulation of metal homeostasis by metal-sensing transcription factors in bacteria. **J. Roe***

- 10:30 – 1415.** Activity of the nickel-responsive transcription factor NikR. **D.B. Zamble**

- 11:00 – 1416.** Creation of a metal-sensor. **N.J. Robinson***

- 11:30 – 1417.** Exploring protein allostery and dynamics in metalloregulatory proteins. **D.P. Giedroc***, J. Braymer

Sheraton Waikiki
Kahuku

Life at Small Copy Numbers (#137)

Organized by: S. Yoshimura, J. Xiao, P. Chen
Presiding: T. Komatsuzaki

- 8:00 opening remark**

- 8:05 – 1418.** Toward deciphering molecular individuality in systems biology. **T. Komatsuzaki***

- 8:35 – 1419.** Modeling timing phenomena in single-cells: From phage-induced lysis to cell-division events. **A. Singh**, K. Ghusinga, J. Dennehy

- 9:05 – 1420.** Conformational motions in protein machines and motors from coarse-grained modeling. **H. Flechsig***

- 9:25 break**

- 9:35 – 1421.** Regulation of the rotational switching of bacterial flagellar motor by binding of an intracellular signaling protein Che. **A. Ishijima**

- 10:05 – 1422.** Directional accuracy in a model of gradient signaling during yeast mating. **E. Roberts**

- 10:35 – 1423.** Cooperative conformational changes of microtubule by kinesin as the mechanism for the spontaneous polarization of intracellular transport in neurons. **Y. Okada***

- 10:55 break**

- 11:05 – 1424.** Lhx2 regulates the timing of b-catenin-dependent cortical neurogenesis. **S. Chou**

- 11:35 – 1425.** Mechanism of influenza virus entry into host cells via calcium signaling-mediated endocytosis. **Y. Fujioka**, A. Nanbo, S. Nishide, Y. Ohba*

- 11:55 closing remark**

Royal Hawaiian
Regency I

Bioorganic Reaction Mechanisms (#224)

Organized by: J. Richard, M. Tanner, C. Easton
Presiding: C.J. Easton

- 8:00 – 1426.** Synthesis and application of cyclic selenides having high-polar functional groups as ER-resident oxidoreductase models. **K. Arai***, M. Iwaoaka

- 8:20 – 1427.** Structure function studies on matrix metalloproteinases (MMPs).

- M.W. Crowder***, K. Makaroff, F. Meng, N. Pas, G. Kuznienski, H. Yang, D. Tierney

- 8:40 – 1428.** Dissecting the mechanisms of endo-acting mannosidases. Z. Hakki, G. Speciale, T. Belz, C. Rovira, G.J. Davies, **S.J. Williams**

- 9:15 – 1429.** Covalent and noncovalent approaches to promote PNA invasion for In vivo applications. **M. Komiya***

- 9:50 – 1430.** Bifunctional molecules containing [12]aneN₃ and fluorescent moieties as effective nonviral gene vectors and transfection mechanism study tool. **Z. Lu**, Y. Gao, Y. Zhang, K. Zhang

- 10:20 – 1431.** Asymmetry of hydrogen bonds in solution. **C.L. Perrin**

- 10:50 – 1432.** Molecular mechanisms of the medicinal thiosulfonates from garlic and petiveria: They are not antioxidants, but lipophilic analogs are. **D. Pratt**

- 11:25 – 1433.** Deciphering and engineering the chemical complexity of cellular microtubules: Insights from structural studies of tubulin modification enzymes. **A. Roll-Mecak***

Royal Hawaiian
Regency III

Function, Chemistry, and Signaling of Glycolipids and Phospholipids (#273)

Organized by: C. Cairo, M. Best, W. Cheng
Presiding: M. Best

*** Principle Author**

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- 8:00** Opening remarks
- 8:00 – 1434.** Remodeling of membrane glycolipids by the human neuraminidase enzymes alters cell migration. **C. Cairo***
- 8:40 – 1435.** Highly efficient preparation of sphingoid bases from glucocerebrosides toward construction of lipids and glycolipids chemical library. **K. Monde***, S.B. Gowda, K. Yamane, A. Nakahashi, M.A. Hammam, T. Taniguchi, A.C. Kumar, S. Usuki, Y. Igarashi
- 9:00 – 1436.** Design of long-lasting peptide anchors for cell surface engineering inspired from natural membrane proteins. **W. Hatanaka***, M. Takeo, R. Tokunaga, M. Kawaguchi, A. Kishimura, T. Mori, Y. Katayama
- 9:20 – 1437.** Cell surface engineering via biorthogonal liposome fusion. **M.N. Yousaf**
- 10:00** Break
- 10:15 – 1438.** Metabolic production of photocrosslinking gangliosides to capture ganglioside-protein interactions. A.M. Wands, A. Fujita, J. Kohler*
- 10:55 – 1439.** Spontaneous phospholipid membrane formation by native chemical ligation. **R.J. Brea***, C.M. Cole, N.K. Devaraj
- 11:15 – 1440.** Protein-glycolipid interactions studied *in vitro* using ESI-MS and nanodiscs: Insights into the mechanisms and energetics of binding. L. Han, E. Kitova, J. Li, S. Nikjah, **J. Klassen***

MTL

Area 8 – Materials & Nanoscience

Tuesday Morning

Hawaii Convention Center

318B

Nanocrystal Synthesis, Characterization, Assembly and Applications (#34)

Organized by: R. Tilley, S. Skrabalak, T. Hyeon, T. Nann, T. Adshiri

8:00 – 1. Some biological applications of nanomaterials, from quantum dots, through polymers, to biosynthesis. **M.A. Green****8:20 – 2.** Facet-dependent properties of inorganic nanocrystals. **M.H. Huang****8:40 – 3.** NMR techniques for characterization of Au nanoparticle surface chemistry. **J.E. Millstone***, L. Marbella**9:00 – 4.** Synthesis of biocompatible fluorescent metal nanoclusters and biomedical imaging. **S. Tanaka*****9:20 – 5.** TEM investigations of particle-mediated crystal growth. **D. Li**, K. Rosso, J.J. De Yoreo**9:40 – 6.** In situ liquid cell STEM of seeded metal nanostructure growth. **R.G. Weiner**, D.P. Chen, R.R. Unocic, S.E. Skrabalak***10:00 – 7.** Self-assembly of gold nanoparticles with a fluorinated surface. **K. Niikura***, J. Wei, N. Sugimura, H. Mitomo, K. Ijiro**10:20 – 8.** Microwave-assisted continuous flow synthesis of CuInS₂ quantum dots. R. Fitzmorris, M. Ahmadi, B. Mangum, J. Kurkin, G. Herman***10:40 – 9.** Formation mechanism of Ag@FeCo@Ag core@shell@shell nanoparticles. **M. Takahashi**, K. Higashimine, P. Mohan, D.M. Mott, S. Maenosono***11:00 – 10.** Novel route for surface modification of superparamagnetic nanoparticles in suspension for biomedical applications. **D.E. Jaskolska***, C. Meledandri**11:20 – 11.** Hybrid NiFe₂O₄ / (Ni,Fe)O particles produced by induction plasma. S. Bastien*, C. Ricolleau, **N. Braidy**Hawaii Convention Center
318A

Conjugated Polymers for Biological Applications (#43)

Organized by: H. Yu, S. Wang, J. Tovar
Presiding: J.D. Tovar, H. Yu**8:00** Opening Address**8:10 – 12.** Applications of conjugated poly-electrolytes in biosensing and disinfection. **K. Schanze****8:50 – 13.** Amphiphilic conjugated block copolymers for single- and two-photon fluorescence imaging. **Y. Tian*****9:10 – 14.** Electropolymerization of functionalized 3,4-ethylenedioxythiophene: Methods, properties, and applications. **S. Luo****9:40 – 15.** Functional conjugated polymers for self-signaling and signal-amplifying biosensors and sensor arrays. **J. Kim*****10:00 – 16.** Optical functional conjugated polymer materials for biomedical applications. **S. Wang*****10:30 – 17.** Preparation of fluorescent conjugated polymer microspheres with monodispersity, bioconjugatability or tunable emission. **L. Fan*****10:50 – 18.** Tris(cyclometalated iridium)-functionalized conjugated oligomers with nonlinear optical properties and bio-applications. **D. Zhao*****11:20 – 19.** Oligofluorene for rapid and specific identification of antibiotics with membrane-disrupting ability. **F. Lu***Hawaii Convention Center
321B

Molecular Adsorption on Metallic Interfaces: Beyond the Cartoons (#102)

Organized by: D. Bizzotto, I. Burgess, H. Yu
Presiding: I.J. Burgess, H. Yu**8:00** Introduction. Optical methods**8:10 – 20.** Super-resolution fluorescence microscopy for understanding and characterising biointerfaces. **J. Gooding**, X. Lu, T. Tabarin, P. Nicovich, V.S. Chand, K. Gaus**8:40 – 21.** Optical and electrochemical methods to probe structure and organization in short chain SAMs. **A.G. Brolo****9:00 – 22.** Exploring the non-homogeneities of DNA mixed self-assembled monolayers by coupling electrochemistry and fluorescence microscopy. **T. Doneux***, A. Meunier, E. Triffaux, C. Buess-Herman**9:30 – 23.** Electrochemically controlled oil droplet reshaping on Au electrode surface in aqueous solution. **T. Sagara***, T. Morooka, Y. Yoshinaga, H. Tahara**9:50 – 24.** Studying the influence of surface crystallography on long and short range organization of DNA self assembled monolayers prepared by thiol exchange on a single crystal gold bead. Z.L. Yu*, J. Casanova-Moreno, **D. Bizzotto****10:10** Break. Probe Microscopy**10:20 – 25.** Thiolated DNA on gold: Single molecule insights enabled by high resolution microscopy. **T. Ye*****10:50 – 26.** Isolation of thiol at electrochemically-controlled ovalene adlayer on Au(111). **S. Yoshimoto*****11:10 – 27.** Multiplicity in adsorption states of self-assembled monolayers on Au(111). **M. Hara*****11:40 – 28.** Interfacial structure and function of nanostructured membranes of newly synthesized phosphorylcholine derivatives. **T. Sawaguchi**Hawaii Convention Center
317A

Design, Synthesis and Applications of Advanced Porous Materials (#111)

Organized by: C. Doonan, M. Dinca, S. Telfer, S. Furukawa, Q. Li

8:00 – 29. Dimensional crossover in coordination frameworks. **H. Kitagawa*****8:30 – 30.** Versatile approach to MOF-polymer mixed-matrix membranes. **S. Cohen**, M. Denny**9:00 – 31.** Catalytic metal-organic frameworks (MOFs): Design and preparation. **O.K. Farha****9:20 – 32.** Photoinduced postsynthetic polymerization of metal-organic framework for the flexible stand-alone membrane. **B. Wang****9:40 – 33.** Following catalytic transformations in MOFs. **C. Doonan***, C. Sumby, A. Burgun**10:00 – 34.** Metal organic frameworks as catalyst and catalyst precursors for C1 chemistry. **A. Olivos**, T. Wezendonk, D. Osadchi*, F. Kapteijn, J. Gascon**10:20 – 35.** Functional organic frameworks as platforms for light-driven hydrogen evolution. **B.V. Lotsch*****10:40 – 36.** Metal-organic frameworks as supporting macromolecular ligands for small molecule reactivity. **M. Dinca****11:00 – 37.** Synthesis, characterization, and catalytic applications of functionalized porous coordination polymers. **H. Choudhary**, S. Nishimura, K. Ebaitani***11:15 – 38.** Photoswitching in thin films of metal-organic frameworks: Optically triggered release of guest molecules. **L. Heinke****11:30 – 39.** Radially expandable metal-organic frameworks. **W. Choe****11:45 – 40.** MOFs as a crystallisation matrix: Structural insights into metal-centred reactions. **W. Bloch**, A. Burgun, C. Coglian, C. Doonan, **C. Sumby**Hawaii Convention Center
316A

Frontier and Perspectives in Molecular Spintronics (#127)

Organized by: M. Yamashita, B. Zhang, H. Tajima, B. Hu, P. Lahti, J. Gao
Presiding: M. Ruben, H. Tada**8:00 – 41.** Frontier of quantum molecular spintronics based on single-molecule magnets: Giant and tunneling magnetoresistances. **M. Yamashita*****8:30 – 42.** Sandwich-type lanthanide single-molecule magnets with tetrathiafulvalene unit: Synthesis, properties, and surface assembly. **J. Zuo****9:00 – 43.** Revealing atomic site-dependent g-factor within a single magnetic molecule via extended Kondo effect. **S. Du****9:30 – 44.** Molecular spins in a quantum box. **M. Affronte*****10:00** Break**10:15 – 45.** Single magnetic molecules studied by LT STM. **Y. Wang****10:45 – 46.** Organometallic spin crossover and single-molecule magnetism. **J. Tao***, C. Wang, X. Yang, F. Liu, L. Zheng**11:15 – 47.** Toward quGuates: Switching of a coupled spin pair in a binuclear Co(II)₂-complex. **M. Ruben**Hawaii Convention Center
319A

Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157)

Organized by: S. Horikoshi, N. Serpone, R. Gupta, Y. Hayashi, M. Ashokkumar, M. Watanabe
Presiding: M. Ashokkumar,

D. Carnaroglio, A.E. Stieglman, K. Suslick

8:00 Opening Remarks**8:05 – 61.** Electrochemical oxidation and production of oxidant species using boron doped diamond films. E. Vieira dos Santos, M. Rodrigo, D. Ribeiro da Silva, **C. Martinez-Hutile*****8:30 – 62.** Photocatalytic activity of sputtered TiO₂ on lightly boron-doped diamond film. **C. Terashima***, R. Hishimura, Y. Sugiyama, K. Nakata, T. Kondo, M. Yuasa, A. Fujishima**8:50 – 63.** Proposal of various application of boron doped diamond electrode. **S. Yoshihara*****9:15 – 64.** Investigation of electrochemical corrosion mechanism in boron-doped diamond electrode. **T. Kashiwada**, T. Watanabe, Y. Einaga**9:30 – 65.** Stability of BDD electrodes in biological conditions. **R. Trouillon*****9:55** Break**9:00 – 51.** Improvement in the gelation properties of fat containing dairy systems through the application of power ultrasound. **J. Chandrapala**, L. Ong, B. Zisu, S. Gras, S. Kentish, M. Ashokkumar**9:15** Ken Suslick**9:15 – 52.** Waste oils treatment in a new ultrasound-assisted mixing device. **D. Boffito***, P. Ruiz Martinez, G.S. Patience**9:30 – 53.** Effect of air sparging on acoustic cavitation oxidation. **Y. Son***, W. Lee, S. Kim**9:45 – 54.** Cavitation in aqueous systems: Exactly what is sonochemistry?. **G.J. Price*****10:00** Brack**10:15** Diego Carnaroglio**10:15 – 55.** Microwave-specific effects on the rates and product distribution of gas-carbon reactions. **A.E. Stieglman**, T. Ferrari**10:30 – 56.** Heterogeneous reactions induced by microwave irradiation: Significant MW effects in catalysis on carbon supported polyoxometalate cluster catalysts and core shell zeolite. **S. Tsubaki**, A. Onda, T. Ueda, E. Suzuki, D. Mochizuki, M. Maitani, Y. Wada**10:45 – 57.** Managing microwave-induced hot spots in heterogeneous catalytic systems. **S. Horikoshi**, N. Serpone**11:00 – 58.** Microwave-solvothermal conversion of glycerin to GTBE using carbon-based catalyst. **S. Uchikado**, Y. Sumigawa, A.T. Qutain, M. Sasaki, T. Kida**11:15** Albert Stieglman**11:15 – 59.** Development of a novel microwave-assisted synthesizer for non-thermal reactions. I. Nagashima, T. Sakuta, **H. Shimizu***, Y. Oki, N. Takahashi**11:30 – 60.** Microwave heating for liquid samples using single-mode microwave resonator. **T. Sumi**, S. HorikoshiHawaii Convention Center
322AB

Electrochemistry on Boron-doped Diamond (BDD) Electrodes (#162)

Organized by: Y. Einaga, S. Park, O. Chailapakul, J. Zhi, T. Kondo
Presiding: O. Chailapakul, Y. Einaga**8:00** Opening Remarks**8:05 – 61.** Electrochemical oxidation and production of oxidant species using boron doped diamond films.E. Vieira dos Santos, M. Rodrigo, D. Ribeiro da Silva, **C. Martinez-Hutile*****8:30 – 62.** Photocatalytic activity of sputtered TiO₂ on lightly boron-doped diamond film. **C. Terashima***, R. Hishimura, Y. Sugiyama, K. Nakata, T. Kondo, M. Yuasa, A. Fujishima**8:50 – 63.** Proposal of various application of boron doped diamond electrode. **S. Yoshihara*****9:15 – 64.** Investigation of electrochemical corrosion mechanism in boron-doped diamond electrode. **T. Kashiwada**, T. Watanabe, Y. Einaga**9:30 – 65.** Stability of BDD electrodes in biological conditions. **R. Trouillon*****9:55** Break

* Principle Author

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10:05 – 66. Development of electrochemical sensor based on boron-doped diamond electrode coupled with paper-based analytical devices. **O. Chaipakul**, W. Siangproh

10:30 – 67. Effects of nanodiamonds' modification with different targeting molecules on cellular uptake profile and consequent impact on cancer cells. **J.F. Zhi***, d. Li, x. Chen, H. Wang

10:55 – 68. Gold modified-boron doped diamond electrode for electrochemical detection of neaminidase. **T.A. Iavandis***

11:15 – 69. Electrochemical detection of influenza virus using hemagglutinin-binding peptide-modified diamond electrode. **M. Ujii***, M. Akahori, T. Matsubara, T. Yamamoto, Y. Einaga, T. Sato

11:30 – 70. Fabrication of boron-doped diamond microelectrodes for local electroanalysis. **D. Kusaka**, T. Kondo, T. Aikawa, M. Yuasa

11:45 – 71. Fabrication of micro flow device using boron-doped diamond for electrochemical analysis. **S. Shibano***, H. Maeda, T. Watanabe, Y. Matsumoto, Y. Einaga

Hawaii Convention Center
320 Theatre

Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223)

Organized by: D. Jiang, W. Wang, W. Zhang
Presiding: D. Jiang, W. Zhang

8:00 Opening remark

8:05 – 72. Recent advances in covalent organic frameworks. **O.M. Yaghi***

8:30 – 73. Amine-tethered porous polymer networks (aPPNs) for carbon capture. **H. Zhou***

8:55 – 74. Porosity of nonporous organic materials. **J.L. Atwood***, H. Kumari, L. Barbour

9:20 – 75. Direct on-surface patterning of a crystalline imine-based covalent organic framework. **F. Zamora***, D. Rodriguez-San-Miguel, A. de la Peña Ruigómez, J. Segura, D. Maspoch, F. Liscio, M. Cavallini, R. Mas-Balleste, D. Gentili

9:35 – 76. Some new metal-organic frameworks with multiple functions. **X. Bu**

9:50 Coffee Break

10:05 – 77. Separation science with cyclodextrin metal-organic frameworks. **J.F. Stoddart**, K.J. Hartlieb, J.M. Holcroft

10:30 – 78. Crystalline, oriented thin films of redox-active covalent organic frameworks for efficient energy storage. **W. Dichtel**

10:55 – 79. Kintting hypercrosslinked micro-porous organic polymer. **B. Tan**

11:20 – 80. Targeted design and applications of porous polymers. **S. Qiu**

11:45 – 81. Effective CO₂ capture by covalent organic polymers through amine binding and N₂ rejection. **H. Patel**, J. Byun, D. Thirion, S. Subramanian, E. Ozdemir, **C.T. Yavuz**

Hawaii Convention Center
321A

Nanomaterials for Nanomedicine (#229)

Organized by: A. Maruyama, D. Lee, R. Narain
Presiding: C. Ahn, M. Ebara, S.K. Hahn

8:00 opening remark

8:05 – 82. Injectable polymeric hydrogels for sustained delivery of proteins. **D. Lee***

8:30 – 83. Smart nanofibers for stick-on anti-cancer treatment. **M. Ebara**

8:55 – 84. Fabrication of water-repellent nanosheets to provide abilities of water retentivity and fixation for tissue imaging. **Y. Okamura***, A. Masuda, K. Okuyama, A. Kotani, Y. Nagase

9:10 – 85. Construction of polymer co-delivery micro- and nanocarriers for pulmonary delivery. **H. Tian***, C. Xu*, X. Chen*

9:25 – 86. Injectable hydrogel system for the delivery of bioactive agents. **S. Lee**, Y. Byun, **C. Ahn***

9:50 – 87. Ureido-functionalized polymers exhibiting UCST-type phase separation under physiological conditions. **N. Shimada***, M. Saito, A. Maruyama*

10:15 – 88. Stem cell/nanoparticle hybrids for targeted cancer therapy. **J. Berlin**

10:30 – 89. Design of dendrimer-gold nanohybrids for biomedical applications. **K. Kono***, T. Hashimoto, X. Li, E. Yuba, A. Harada

10:45 Break

10:55 – 90. Redox injectable gels for local inflammation treatments. **Y. Nagasaki**

11:20 – 91. Multistimuli-responsive nanoparticles for anticancer and antiinflammation therapy. **S. Jon**

11:45 – 92. Preparation of thermoresponsive nanoparticles as biomaterials. **A. Kikuchi***, T. Matsuyama, T. ASOH, T. Suzuki, R. ISHIHARA

Hawaii Convention Center
316B

The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347)

Organized by: M. Srinivasarao, A. rey, H. Jung

8:00 – 93. Chiro-optical materials inspired by the handed single gyroid structure in green butterflies. **G.E. Schröder-Turk***

8:35 – 94. Self-assembly and function of butterfly proboscis. **K. Kornev**

9:10 – 95. Nanoscale surface wrinkling in plant-based plywood with hydration-induced chiral gradients. **P. Rofouie***, D. Pasini, A. Rey

9:35 – 96. Giant spiral structure formed by microtubules through their partial depolymerization and subsequent dynamic ordering. **K. Shikinaka***, H. Kudoh, S. Mori, A. Kakugo, R. Kawamura, J. Gong, H. Masunaga, K. Shigehara

10:00 Session Break

10:20 – 97. Polymer microparticles with biomimetic pollen-like surface structures. **O. Karthaus***, P. Polzin, P. Acker

10:45 – 98. Dynamics of active colloids in confined systems. **J. Molina***, J. Delfau*, R. Yamamoto, M. Sano

11:10 – 99. Biophysical characterization of reflectin isoforms from squid and cuttlefish. **L. Phan**, R.W. Walkup IV, D.D. Ordinario, **A.A. Gorodetsky***

11:35 – 100. Self-healing films with deliquescent salt via Layer-by-Layer self-assembly method and controlling their functional properties. **S. Shiratori**, T. Taniguchi

Hawaii Convention Center
314

Safety and Sustainability of Nanotechnology (#404)

Organized by: Y. Zuo, J. Ferri, C. Chen, J. Loo, S. Mylon
Presiding: C. Chen, D.T. Leong, A. Nel, Y. Zuo

8:00 Welcome

8:05 – 101. Use of alternative test strategies, predictive toxicological approaches, and categorization to expedite decision analysis of nanomaterial safety. **A. Nel***

8:35 – 102. Nanotechnology and sustainability: Making the connection. **B.P. Karn***

9:00 – 103. Elucidation of immunotoxicity of nanoparticles for developing the sustainable nanotechnology. **Y. Yoshioka***, K. Higashikura, Y. Tsutsumi

9:25 Coffee Break

9:35 – 104. Endoplasmic reticulum stress is an earlier biomarker for nanotoxicological evaluation. **C. Chen***

10:00 – 105. Unexpected noncytotoxic nanoparticles effects on endothelial and epithelial cells. **D.T. Leong***

10:25 – 106. Public safety perception and sustainability of nanotechnology. **G. Wang***

10:50 – 107. Interaction of nanoparticles with cells: The importance of the physico-chemical properties and dose-metrics as a basis for nanotoxicology assessment. **N. Feliu***, R. Alvarez-Puebla, W. Parak

11:10 – 108. Effect of polyethylene glycol on the in-situ adsorption of human serum albumin on nanoparticles surface. **B. Pelaz**, P. del Pino, R. Hartmann, W. Parak

Hawaii Convention Center
316C

Single-Molecule Function and Measurements (#408)

Organized by: T. Ogawa, H. Tada, S. Park, P. Weiss
Presiding: T. Ogawa, H. Tada

8:00 Break

8:10 Remarks

8:15 – 109. Low temperature mechanically controllable break junction of oligothiophene molecular wires. T. Shimomise, F. Jimmy, S. Tanaka, T. Ohto, R. Yamada, **H. Tada**

8:45 – 110. Simulated force-conductance spectroscopy of hydrogen-bonded bimolecular complexes. A. Pirrotta*, G.C. Solomon, **I. Franco**

9:05 – 111. Single molecular devices using supermolecules. **M. Kiguchi**

9:35 – 112. Hybrid density functional study on electron transport through π-stack molecular junctions for high conductance. **T. Tada***

10:05 Break

10:20 – 113. Probing spinterface in single molecular junctions by thermoelectric measurements. **R. Yamada***, S.K. Lee, T. Ohto, H. Tada

10:40 – 114. First-principle study of thermo-electric transport through single molecule junctions. **M. Buerkle**, Y. Asai

11:00 – 115. Quantum transport theory for the current induced local heating and the current noise. **Y. Asai***

11:30 – 116. On the utilization of anti-Stokes/Stokes ratios in single-molecule surface-enhanced Raman spectroscopy for nanoscale thermometry. **E.A. Pozzi***, A.B. Zrimsek, M.C. Hersam, R.P. Van Duyne

Hawaii Convention Center
319B

Self-assembled Biofunctional Nanomaterials (#433)

Organized by: R. Nagarajan, K. Sakurai, H. Chen

8:00 – 117. Characterization of functional nanomaterials for emerging biomedical applications. **D. Tsai**

8:30 – 118. Anisotropic gold nanocrystal growth directed by the interior cavity of a self-assembled peptide nanoarchitecture. **K. Tomizaki***, K. Kishioka, M. Kasuno, T. Imai

8:50 – 119. Controlled assembly of biocompatible metallic nanoaggregates using a small molecule crosslinker. **J. Berlin**

9:10 – 120. Luminescent gold nanoparticles: An antifouling surface ligand for minimizing nonspecific serum protein adsorption. **J. Zheng***

9:30 – 121. Computational approaches to investigating thio- and amino-based adsorbents on a gold surface -- a density functional theory (DFT) study. **C. Ting**

9:50 Break

10:00 – 122. Reaction-based Indicator displacement assay (RIA). **T.D. James**

10:30 – 123. Out-of-equilibrium biomimetic systems by dynamic and dissipative self-assembly. **J. van Esch***, R. Eelkema, G. Koper, W. Hendrikse, J. Boekhoven, J. Poolman, A. Olive, M. Lovrak, C. Maity

11:00 – 124. Supramolecular hydrogels self-assembled from ultrashort tetraphenylethylene-capped peptides. **C. Huang**

11:20 – 125. Self-assembling behavior of tranexamic acid cetyl hydrochloride in aqueous solution. **Y. Yamashita***, T. Ohta, M. Miyamoto, K. Sakamoto

11:40 – 126. Self-assembled glycopolyptide copolymer nanoparticles: Bioactivity and multivalency. **S. Lecommandoux**

Tuesday Afternoon

Hawaii Convention Center
318B

Nanocrystal Synthesis, Characterization, Assembly and Applications (#34)

Organized by: R. Tilley, S. Skrabalak, T. Hyeon, T. Nann, T. Adshiri

13:00 – 127. Silicon nanocrystal surface chemistry: We all thought we had if figured out...but did we? **J. Veint***

13:40 – 128. Supercritical route for functional nanoparticles. **T. Adschar***

14:00 – 129. Precursors for the deposition of inorganic nanostructures: Adapting design for the technique. **L. McElwee-White***

14:20 – 130. Enhanced nanoparticle size control by extending LaMer's mechanism. **D. Huber***, E. Vreeland, B. Hance, J. Watt, C. Rinaldi

14:40 – 131. Synthesis and characterization of gold-palladium bimetallic nanoparticle catalysts. **S. Cheong***

15:00 – 132. Effect of seed age on gold nanorod formation: A microfluidic, real-time investigation. **J. Watt**, B. Hance, R. Anderson, D. Huber

15:20 – 133. "Living" nanocrystals: Preparation and precise size control of metal oxide nanocrystals via living chain polycondensation. **J. Hutchison***, A.W. Jansons, B.M. Crockett, M.C. Sharps, L.K. Plummer

15:40 – 134. In situ synchrotron X-ray study of the formation mechanism of multicomponent nanoparticles. **S. Kwon**, G. Krylova, P. Phillips, R. Klie, S. Chattopadhyay, T. Shibata, E. Bunel, y. Liu, V. Prakapenka, B. Lee, E.V. Shevchenko

16:00 – 135. Palladium-based octopodal nanocrystals formed via copper-assisted growth. **M. Hartley**, R.G. Weiner, S.E. Skrabalak*

16:20 – 136. Site-selective electrochemical fabrication of organic nanocrystals: Electromagnetic device applications and their properties. **H. Hasegawa**

16:40 – 137. Preparation and evaluation of magnetic Co-Ni nanoparticles in recyclic use for selective hydrogenation of CNB. **O. Nakagoe**, H. Kataoka, Y. Kido, S. Tanabe*

Hawaii Convention Center
318A

Conjugated Polymers for Biological Applications (#43)

Organized by: H. Yu, S. Wang, J. Tovar
Presiding: J.D. Tovar, S. Wang

13:00 – 138. Interfacing with the brain using organic electronics. **G. Malliaras**

13:40 – 139. Organic conductive nanomaterials: From solar cells to cancer cells. **H. Yu***

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14:10 – 140. Biomolecular interactions at the biomolecule-PEDOT interface: Insights from first-principles calculations.

A.M. Sultan*, Z.E. Hughes, T.R. Walsh
14:30 – 141. Organic bioelectronics for cell sensing sorting and drug release.
P. Chen*

15:00 – 142. Functional conjugated polymers: towards new materials for biomedical applications. J. Travas-Sejdic

15:30 – 143. Graphene oxide-conjugated polymer hybrid materials for detection and function regulation of calmodulin.

C. Xing, H. Yuan, J. Qi, Y. Zhan
15:50 – 144. Organic bioelectronics create ionic microenvironments mimicking inflammation and infection for elucidating activation dynamics of C-reactive protein.

T. Goda*, Y. Miyahara
16:20 – 145. Stimulating regenerative biological processes using organic bionics.

G.G. Wallace*

Hawaii Convention Center
321B

Molecular Adsorption on Metallic Interfaces: Beyond the Cartoons (#102)

Organized by: D. Bizzotto, I. Burgess, H. Yu, T. Sagara, H. Yang
Presiding: D. Bizzotto, T. Sagara, H. Yang

13:00 Introduction. SAM characterization
13:10 – 146. Redox behavior of the $[Fe(CN)_6]^{3-/4-}$ complex entrapped onto ionic liquid-modified electrode as observed by SEIRAS measurement.

T. Kitagawa*, T. Inomata, T. Ozawa, H. Masuda, K. Motobayashi, M. Osawa
13:30 – 147. Manipulation of biomolecular functions at electrode surfaces via surface modification. X. Xia*

14:00 – 148. Electrochemical heterogeneity in "ideally behaved" redox self-assembled monolayers. H. Yu

14:20 Break. Nanoparticles & QDs

14:30 – 149. Exciton transport and dissociation in quantum dots, rods and platelets. T. Lian*

15:00 – 150. Comparison of silver nanoparticles prepared by physical and chemical synthetic methods using the same protective agents. T. Ienaga*, Y. Nakahara, K. Kimura

15:20 – 151. Decoration of conductive surfaces with amine-terminated dendrimers encapsulating catalytic nanoparticles. J. Kim*

15:50 – 152. Homogeneous and heterogeneous formation of anisotropic nanoparticles using pyridine derivatives as stabilizers. B. Dancer, S. Simon, B. Unni, I.J. Burgess*

16:10 – 153. Quinonyl glycosides functionalized quantum dots for sensing. W. Ma, X. He, Y. Long*

Hawaii Convention Center
317A

Design, Synthesis and Applications of Advanced Porous Materials (#111)

Organized by: C. Doonan, M. Dinca, S. Telfer, S. Furukawa, Q. Li

13:00 – 154. Using efficient computational simulations to accelerate development of diffusion-selective MOFs for chemical separations. D. Sholl*, J. Camp, D. Nazarian, R. Verploegh, K. Jayachandrababu, S. Nair

13:30 – 155. Flexibility and phase transitions in metal-organic frameworks. A.K. Cheetham*

14:00 – 156. Structural and dynamical studies of small molecules adsorbed in MOFs. C. Brown

14:20 – 157. Carbon dioxide (CO_2) capture in the presence of water vapour in PCPs. I.A. Ibarra*

14:40 – 158. Porous metal-organic materials for gas storage and selectivity. S. Yang

14:55 – 159. Mesoporous metal-organic frameworks: New host for large molecules. H. Deng*

15:10 – 160. Metal organic frameworks for energy and environmental applications: What we learned from molecular modeling. R. Babarao, M.R. Hill, A. Thornton, A.J. Hill, C. Doonan, C. Sumby, D.M. D'Alessandro

15:25 – 161. Assembly of porous MOFs materials for gas storage and separation applications. Y. Liu, Q. Huo

15:40 – 162. Characterization of heat treated rho-ZMOF via N_2 adsorption.

A. Sirkecioglu*, C. Oral, G. Isilay Ozturk, B. Tantekin-Ersolmaz

15:55 – 163. Chiral coordination frameworks for enantioselective separations.

S.A. Boer, Y. Nolyachai, C. Kulasing, C.S. Hawes, P.J. Marriott, D. Turner*

16:10 – 164. Water/alcohol vapor separation using flexible 2D Mg(II) coordination polymer with isonicotinic acid N-oxide ligand.

R. Ochi*, S. Noro, Y. Kamiya, K. Kubo, T. Nakamura

16:25 – 165. Engineering defects in quaternary metal-organic frameworks.

J.J. Pak*, S. Telfer, S.J. Lee, L. Liu, C. Richardson

16:40 – 166. Freestanding conjugated microporous polymer nanomembranes for gas separation. M. Tsotsalas*, P. Lindemann, H. Gleimann, C. Woell

Hawaii Convention Center
316A

Frontier and Perspectives in Molecular Spintronics (#127)

Organized by: M. Yamashita, B. Zhang, H. Tajima, B. Hu, P. Lahti, J. Gao
Presiding: K. Awaga, B. Hu

13:00 – 167. Lanthanides-TTF complexes: Correlation between SMM and luminescence. L. OUAHAB

13:10 – 168. Molecular magnetic conductor. B. Zhang*, D. Zhu

14:00 – 169. From magnetic molecules to molecular spintronic devices.

E. Coronado*, J. Baldoví, W. Cañón, A. Gaña, S. Gómez-Miralles, A. Bedoya-Pinto, L. Hueso

14:30 – 170. DFT-D study on geometric and electronic structures of double-decker bis(phthalocyanato)terbium(III) complex. Y. Kitagawa*, K. Katoh, M. Asaoka, K. Miyagi, T. Takebayashi, M. Yamashita, M. NAKANO

14:55 Break

15:05 – 171. Switching and sensing spin states of metallo-porphyrin in bimolecular reactions on Au(111) using scanning tunneling microscopy. H. Kim , Y. Chang , S. Lee , Y. Kim , S. Kahng

15:25 – 172. Engineering the exchange coupling at the molecule/electrode interface in molecular spintronic devices. T. Mallah*, V. Campbell

15:55 – 173. Versatile electric and magnetic properties of radical-anion salts with multidimensional crystal structures.

K. Awaga*

16:25 – 174. Electronic transport phenomenon through organic spin-containing molecules. J. Veciana

Hawaii Convention Center
319A

Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157)

Organized by: S. Horikoshi, N. Serpone, R. Gupta, Y. Hayashi, M. Ashokkumar, M. Watanabe
Presiding: J. Hihni, S. Horikoshi, G.J. Price

13:00 Jean-Yves Hinh

13:00 – 175. Applications of ultrasound technology in crystallization and atomization.

S. Nii

13:15 – 176. Shock driven atomic movements in ultrasonically treated metal alloys: Formation of mesoscopic composite metal catalysts. D.V. Andreeva*

13:30 – 177. Synthesis of metal nanoparticles in aqueous solutions by using sonochemically formed reducing radicals. K. Okitsu

13:45 – 178. Ultrasound cavitation based synthesis of doped platinum catalyst for fuel cell application. S.H. Sonawane*, P.L. Suryawanshi, R. P.

14:00 – Gareth Price

14:00 – 179. Comparing lactose nucleation in batch and continuous sonocrystallization for dairy manufacturing. B. Zisu

14:15 – 180. Sonosynthesis of hollow/porous metal oxide microspheres.

M. Zhou*, S. Tan, M. Ashokkumar
14:30 – 181. Development of anodic substitution reaction system using tandem acoustic emulsification.

Y. Ogawa, H. Tateno, K. Nakabayashi, M. Atobe

14:45 – 182. Ultrasonic technology for food processing applications.

M. Ashokkumar

15:00 Brack

15:15 – 183. Microwave accelerated steam distillation from peel and flowers of *Citrus natsudaidai* Hayata.

A. Kurano*, M. Sasaki, A.T. Quitain, T. Kida

15:30 – 184. Sustainable and highly competitive chemical processes under microwave irradiation.

D. Carnaroglio*, L. Rotolo, E. Calcio Gaudino, G. Cravotto

15:45 – 185. Materials processing under microwave non-equilibrium reaction field.

H. Takizawa*, J. Fukushima, Y. Hayashi

Hawaii Convention Center
322AB

Electrochemistry on Boron-doped Diamond (BDD) Electrodes (#162)

Organized by: Y. Einaga, S. Park, O. Chailapakul, J. Zhi, T. Kondo
Presiding: T. Kondo, j.F. ZHI

13:00 – 186. Anodic treatment of aryls using BDD electrodes.

S.R. Waldvogel*

13:30 – 187. Electrochemical reduction by means of boron-doped diamond electrode.

T. Saitoh*, T. Kojima, R. Obata,

Y. Einaga, S. Nishiyama

13:55 – 188. Reduction of carbon dioxide at boron-doped diamond.

K. Nakata*

14:20 – 189. Sensitive electrochemical detection at screen-printed diamond electrode by microelectrode effect.

T. Kondo*, I. Udagawa, T. Aikawa,

I. Shitanda, Y. Hoshi, M. Itagaki,

M. Yuasa

14:40 – 190. Novel boron-doped diamond electrode on paper-based analytical device (BPAD) for adsorptive stripping voltammetric determination of trace copper.

W. Siangproh, S. Chaiyoo, O. Chailapakul

15:00 – 191. Application of Pt/boron-doped diamond powder prepared by the nano-capsule method to fuel cell cathode catalyst support.

M. Kikuchi*, T. Kondo,

T. Aikawa, M. Yuasa

15:15 Break

15:25 – 192. Surface chemical modification of nanodiamond by thermal reaction with alkenes.

A. Ito, T. Kondo, T. Aikawa,

M. Yuasa

15:40 – 193. High speed synthesis of boron-doped diamond by solution plasma.

R. Hishimura, Y. Harada, C. Terashima,

H. Uetsuka, T. Kondo, M. Yuasa,

A. Fujishima*

15:55 – 194. Influence of sp^2 -bonded carbon impurities in moderately and heavily boron-doped diamond for wastewater treatment and ozonized water production.

T. Watanabe*, Y. Einaga

16:15 – 195. Influence of crystal orientation on the electrochemical properties in boron-doped diamond electrodes.

T. Matsui*, T. Watanabe, Y. Einaga

16:30 – 196. Semiconductor-water interfaces investigated by first principles calculations of boron doped diamond.

Y. Tateyama*, Z. Futer, T. Watanabe,

Y. Einaga

Hawaii Convention Center
320 Theatre

Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223)

Organized by: D. Jiang, W. Wang,
W. Zhang
Presiding: J.J. Lavigne, W. Wang

13:00 – 197. Boronic ester-based porous materials: Chemical approaches to control ester stability and guest recognition properties.

J.J. Lavigne*

13:25 – 198. Functional microporous polymer networks for catalysis and energy applications.

A. Thomas

13:50 – 199. Covalent organic frameworks as a material platform for challenging energy issues.

D. Jiang*

14:15 – 200. Preparation and application of functional conjugated microporous polymers.

S. Ren*

14:30 – 201. Exploration of synthetic tricks for conjugated microporous polymers (CMPs): Controllable preparation of CMP-based microspheres, fibers, films, and organogels.

J. Guo

14:45 Coffee Break

15:05 – 202. Functional porous organic polymers and related materials.

J. Hupp*

15:30 – 203. Constructing covalent organic frameworks for catalysis.

W. Wang, Z. Li,

H. Xu, W. An

15:55 – 204. Novel porous molecular solids.

C. Doonan*, A. Burgun

16:20 – 205. Pillar[n]arene-based supramolecular organic frameworks for highly selective sorption and separation of CO_2 and C_2H_2 .

L. Tan, W. Zhang*, Y. Yang*

16:45 – 206. Reactive interface-assisted co-assembly to monodisperse hollow ordered mesoporous polymeric nanospheres and their functional derivatives.

Y. Liang, R. Fu, M. Zhang, D. Wu

Hawaii Convention Center
321A

Nanomaterials for Nanomedicine (#289)

Organized by: A. Maruyama, D. Lee, R. Narain
Presiding: Y. Byun, X. Chen, J. Kizhakkedathu

13:00 – 207. Intelligent and integrated nanosystems for antitumor drug delivery.

X. Chen, Z. Tang, C. Xiao, J. Ding

13:25 – 208. Light mediated use of copper(II) and disproportionation of copper(II) to achieve excellent living polymerisation of acrylamides and acrylates for nanomedicine.

D. Haddleton

13:50 – 209. Rational design of latent ratio-metric fluorescent pH probes based on self-assembled SNARF derivatives.

E. Nakata*, T. Morii

14:05 – 210. Therapeutic glycol chitosan nanoparticles for heterogeneous tumors.

K. Kim

14:30 – 211. Design and development of multifunctional polyether dendritic polymer-based long acting polymeric therapeutics.

J. Kizhakkedathu*, R. Shenoi,

M. Imran ul-haq, J.L. Hamilton, B. Lai,

S. Abbina

* Principle Author

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- 14:55 – 212.** Biodegradable polymeric micelles stabilized and functionalized by coating with polyion complex. **Y. Ohya***, Y. Morimoto, A. Takahashi, A. Kuzuya
15:10 Break
15:25 – 213. Nanoshielding of pancreatic islets for the prevention of immune reactions in allo-transplantation. **Y. Byun**
15:50 – 214. Synthetic polymeric biomaterials to undertake siRNA delivery to leukemic cells. **H. Uludag***
16:15 – 215. Immune-complement-mimicking anticancer therapeutic design: Self-luminative light-driven therapeutic cassette for solid tumour regression. **S. Um***, S. Shin
16:30 – 216. Cyclodextrin-threaded biocleavable polyrotaxanes for the therapy of lysosomal storage disorders. **A. Tamura, N. Yui***

Hawaii Convention Center
317B

Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery (#314)

- Organized by:* J. Schrier,
C. Amador-Bedolla, S. Iwata, T. Woo
Presiding: C. Amador-Bedolla, S. Iwata,
J. Schrier, T. Woo
- 13:00** Introductory Remarks
13:05 – 217. On lesson from material databases. **Y. Shikano***
13:45 – 218. Materials informatics for materials design. **A. Troshpa***
14:15 – 219. Data and knowledge structure for materials integration. **T. Ashino***
14:45 Break
15:00 – 220. Discovery of optimal zeolites and metal-organic frameworks for challenging separations and chemical conversions through predictive materials modeling. **J.I. Siepmann**, P. Bai,
M.W. Deem, E. Haldoupis, K. Vogiatzis,
L. Gagliardi
15:30 – 221. Accurate machine learning recognition of high performing materials for CO₂ capture. **T. Woo**
16:00 – 222. ChemML - a machine learning and informatics toolbox for the chemical and materials sciences. **J. Hachmann***

Hawaii Convention Center
316B

The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347)

- Organized by:* M. Srinivasarao, A. rey,
H. Jung
- 13:00 – 223.** Bio-inspired multimodal tactile electronics using hierarchically engineered carbon nanotube microfabrics. **S. Kim, S. Park, H. Lee, M. Kang, D. Kim***
13:25 – 224. Rheological anf flow modeling of nanocrystalline cellulose aqueous suspensions. **D. Greco***, N. Noroozi
14:00 – 225. Hydrogel actuator based on mussel adhesive protein chemistry. **B.P. Lee***
14:25 Session Break
14:45 – 226. Modeling cell motility and mitosis using complex fluids models involving active matter. **Q. Wang***, J. Zhao, X. yang
15:20 – 227. Nanoparticle-induced cellular aggregates. G. Beaune, B. Brunel,
F. Brochard-Wyart, **F. Winnik***
15:45 – 228. Mixed mode interactions in hydrogels tune hydrophobic crosslinking and selective transport. **W.G. Chen**,
S. Grindly, N. Holten-Andersen,
K. Ribbeck*

Hawaii Convention Center
314

Safety and Sustainability of Nanotechnology (#404)

- Organized by:* Y. Zuo, J. Ferri, C. Chen,
J. Loo, S. Mylon
Presiding: T. Liedl, S. Liu, J. Yang,
Y. Zhao

- 13:00 – 229.** Chemical mechanisms of inorganic nanomaterials toxicity. **Y. Zhao**
13:30 – 230. NLRP3 inflammasome activation induced by engineered nanomaterials: The critical role of lysosomes. **T. Xia**
13:55 – 231. Silver nanoparticles repress hemoglobin transcription through an epigenetic mechanism: Altering the methylation status of histone 3. **S. Liu**
14:20 – 232. Physicochemical properties of PEGLylated gold nanoparticles: Impact on cell fitness. **P. del Pino***, W. Parak
14:40 Coffee Break
14:50 – 233. Selective release system based on mesoporous silica nanoparticle. **W. Wang, Y. Wen, Y. Li, X. Jiao, W. Gui, X. Zhang***
15:15 – 234. Nanomechanical mapping of cellular migration. **X. Chen***
15:40 – 235. DNA self-assembly for biomedical applications. **T. Liedl**
16:05 – 236. Conductive bacterial nanowires: Fundamentals and applications for environmental and energy sustainability. **J. Yang***
16:30 – 237. Assessing nanomaterial safety at the benchtop. **B.D. Gates***, S. Rubino,
K. Cadieux, M.T. Paul, B. Lute, F. Orfino,
J. Zhou

Hawaii Convention Center
316C

Single-Molecule Function and Measurements (#408)

- Organized by:* T. Ogawa, H. Tada,
S. Park, P. Weiss
Presiding: T. Asai, S. Kasai
- 13:00 – 238.** Fluctuation-induced dynamics and information transfer in nonlinear nanodevices and molecular devices. **S. Kasai***, Y. Abe, S. Inoue, K. Shiota, M. Sato
13:30 – 239. Molecular characterization using current noise measurement of carbon nanotubes device. **A. Setiadi**, H. Fujii,
M. Akai-Kasaya*, S. Kasai, Y. Kanai,
K. Matsumoto, Y. Kuwahara
13:50 – 240. Stochastic resonance in molecular network systems. **T. Matsumoto***
14:10 – 241. Neuron-like signal generation and its chaotic analysis of single-walled carbon nanotube and redox nanoparticle complex. **H. Tanaka***
14:40 – 242. Cooperative functions in engineered nanosystems: From supramolecules to metamaterials. **Y. Zheng**
15:10 Break
15:25 – 243. Molecules in circuits: New electronics for audio processing. **R.L. McCreary***, A. Bergren, N. Pekas,
B. Szeto, L. Zeer-Wanklyn, M. Semple
15:55 – 244. Effect of metal work function on large-area molecular junctions with single-layer graphene top contacts. **M. Yamaguchi**, T. Ikuta, Y. Kanai,
T. Ohta, R. Yamada, Y. Ohno,
K. Maehashi, K. Matsumoto, H. Tada
16:15 – 245. Coulomb-blockade transport in low-dimensional conjugated conductive polymers. **M. Akai-Kasaya***, S. Nagano,
T. Mitani, Y. Kuwahara
16:35 – 246. High yield fabrication of gold nanoparticle assemblies on DNA origami templates. **R. Pandey***, T. Ye, G.R. Abel,
H. Tanaka

Hawaii Convention Center
319B

Self-assembled Biofunctional Nanomaterials (#433)

- Organized by:* R. Nagarajan, K. Sakurai,
H. Chen
- 13:00 – 247.** Surface functionalized polymer vesicles: Toward new properties and functions. **E.R. Gillies***, A. Nazemi,
J.T. McIntosh
13:20 – 248. Anion transport across varying lipid membranes. **P. Gale**
13:50 – 249. Water-soluble polyion complex (PIC) micelles covered with phosphoryl-choline and galactose shells. **S. Yusa***,
R. Enomoto, O. Yukie, K. Ishihara

- 14:20 – 250.** Self-assembling and micellization characteristics of well-defined lipid-mimic brush polymers. **M. Ree***, J. Kim,
K. Kwon, J. Lee, Y. Kim, B. Ree, K. Jin,
Y. Sanada, K. Sakurai
14:50 – 251. In situ block copolymer self-assemblies via RAFT aqueous dispersion polymerization of MEA using PEO-macro CTA. **A. Bin Ma Radzi**, S. Sugihara,
S. Ida, t. kikukawa, Y. Maeda
15:10 – 252. Self-assembly of biological lipids and liquid crystalline droplets. **N. Abbott**
15:40 – 253. Rational design of naphthalimide-capped peptides with aggregation-induced emission characteristics. **Y. Huang***
16:00 – 254. Surfactant-like peptides leading to self-assembled structures. **T. Imura***
16:20 – 255. Protein-shell and polymer-core nanoball. **H. Paik**
16:40 – 256. Solution self-assembly of protein-polymer conjugates. **R. Nagarajan**

Wednesday Morning

Hawaii Convention Center
318A

Conjugated Polymers for Biological Applications (#43)

- Organized by:* H. Yu, S. Wang, J. Tovar
Presiding: S. Wang, H. Yu
- 8:00 – 257.** Dendritic polyglycerols as dual modal imaging agent for EGF-receptor mediated tumor targeting. **K. Pant***,
K. Zarschler, R. Bergmann, J. Pietzsch,
H. Stephan
8:20 – 258. π-Conjugated systems based on small molecules and polydiacetylenes for their sensing and antibacterial activity. **J. Yoon***
8:50 – 259. Chemo-/biosensing and imaging based on luminogens with aggregation induced emission. **D. Zhang***
9:30 – 260. Carving supramolecular conjugated pi-ways into biomaterials via peptide self-assembly. **J.D. Tovar***
10:00 – 261. Fluorescent conjugated polymers as sensors, therapeutics, and biocatalysis. **P.K. Iyer***, B. Muthuraj,
S. Hussain, A. Hussain Malik, A. Tanvar,
S. Chowdhury
10:20 – 262. Bioinspired synthesis and characterization of organic nanowires. **A.A. Gorodetsky**
10:50 – 263. Comparing sol-gel entrapped structure-switching DNA and RNA aptamers as biosensing materials. **C.Y. Hui**,
P. Lau, Y. Li, J.D. Brennan*
11:10 – 264. Engineering biointerface with controlled cell adhesion towards cancer detection. **S. Wang***

Hawaii Convention Center
321B

Molecular Adsorption on Metallic Interfaces: Beyond the Cartoons (#102)

- Organized by:* D. Bizzotto, I. Burgess,
H. Yu, T. Sagara, H. Yang
Presiding: D. Bizzotto, H. Yu

- 8:00** introduction
8:10 – 265. DNA nanotechnology-based approach for the development of electrochemical DNA sensors. **C. Fan**
8:40 – 266. Indium-tin oxide electrodes for sensitive and reproducible electrochemical biosensors. **H. Yang**
9:00 – 267. Enzyme adsorbed nanostructure ITO electrode for developing drug metabolism biosensing devices. **O. Niwa***,
K. Yoshioka , S. Shiba, S. Ishihara,
T. Kamata, D. Kato
9:30 – 268. Methylsorb: A simple method for quantifying DNA methylation using DNA-gold affinity interaction. **A. Sina***,
L.G. Carrascosa, S. Dey, M. Shiddiky,
M. Trau
9:50 break
10:00 – 269. Diazonium derived vs. thiol derived molecular layers on gold electrodes: Structure and stability. **M. McDermott***,
L. Laurentius, A. Kebede, D. Shewchuk

- 10:30 – 270.** Suppression of bimolecular decay of reactive triplet carbene by immobilization through self-assembled monolayer of tripod-shaped trithiol on gold. **T. Kitagawa***, K. Hirai, K. Nishiaki,
K. Ueda
10:50 – 271. Adsorption energy calculations using long-range corrected density functional theory between CO and metal system. **J. Song***, K. Hira
11:10 – 272. Strengthening of the copper/epoxy resin interface with an amino-functional polymer. **P. Nothdurft***,
S. Feldbacher, W. Kern

Hawaii Convention Center
317A

Design, Synthesis and Applications of Advanced Porous Materials (#111)

- Organized by:* C. Doonan, M. Dinca,
S. Telfer, S. Furukawa, Q. Li

- 8:00 – 273.** Metal-organic frameworks for electronic and photonic device applications. **M.D. Allendorf***, M. Foster,
F. Léonard, C. Spataru, V. Stavila,
A. Talin, C. Schneider, R. Fischer,
H. Mieno, C. Adachi

- 8:30 – 274.** Ordered defects in metal-organic frameworks by crystal engineering. **B. Tu**,
Q. Li
8:50 – 275. Melting, and glassy MOFs with porosity and ion conductivity. **S. Horike**

- 9:10 – 276.** Functional nanoporous metal oxides and graphenes derived from metal-organic frameworks. **H. Moon***
9:30 – 277. Partially interpenetrated metal-organic frameworks (MOFs). **S. Telfer**

- 9:50 – 278.** Thin films of metal-organic frameworks: The search for new deposition methods. **I. Stassen**,
M. Timmermans, M. Styles, H. Van Gorp,
S. De Feyter, P. Falcaro, D. De Vos,
P. Vereecken, **R. Ameloot***

- 10:10 – 279.** Engineering pore surface of metal azolate frameworks for efficient gas separation. **J. Zhang***

- 10:30 – 280.** Metal-organic frameworks as platform to arrange and protect single-molecule magnets in multidimensional arrays. **M. Wriedt**, J. Pyser, D. Aulakh,
X. Zhang, A. Yakovenko, K. Dunbar

- 10:45 – 281.** Where is the oxygen? Crystaline sponge method applied to the structural analysis of sesquiterpene oxidation products. **N. Zigon***, M. Hoshino,
S. Yoshioka, Y. Inokuma, M. Fujita
11:00 – 282. Top-down fabrication of metal-organic frameworks nanoparticles with hollow structure. **M. Hu***

- 11:15 – 283.** Assembly, disassembly, and reassembly as a strategy for the construction of mixed-metal organic frameworks. **S. Baudron***, A. Béziau, M. Hosseini

- 11:30 – 284.** Crystalline sponge method for synthetic organic chemistry. **Y. Inokuma***, M. Fujita
11:45 – 285. Macrostructured quartz films on silicon obtained via processing driven phase separation. **G.L. Drisko***,
A. Carretero-Genevier, M. Gich,
J. Gázquez, D. Grossio, C. Boissière,
J. Rodríguez-Carvajal, C. Sanchez

*** Principle Author**

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TECHNICAL PROGRAM

Hawaii Convention Center
316A

Frontier and Perspectives in Molecular Spintronics (#127)

Organized by: M. Yamashita, B. Zhang, H. Tajima, B. Hu, P. Lahti, J. Gao
Presiding: V.A. DEDIU, I.A. Hümmelgen

8:00 – 286. Enhanced magnetic field effects on an indoletrimer-based spin-polarized donor due to its 3-fold rotational symmetry. **M.M. Matsushita***, Y. Ishii, K. Awaga

8:20 – 287. Magnetoresistance in organic field-effect transistors and diodes. **H. Tada***

8:50 – 288. Magnetoresistance in organic spintronic devices: Real and imaginary effects. **V.A. DEDIU***, A. Riminiucci, I. Bergenti, P. Graziosi, M. Calabucci, R. Checchin

9:20 – 289. Annealing effect on tunneling anisotropic magnetoresistance in organic spin valves. **C. Miyahara***, T. Kamiya, H. Tada

9:40 Break

9:55 – 290. Spin current in organic semiconductors. **S. Watana**

10:25 – 291. Impurity-band transport in organic spin valves. **Z. Yu***

Hawaii Convention Center
322AB

Mechanically Responsive Materials (#153)

Organized by: P. Naumov, T. White, B. Kahr, Y. Yu
Presiding: C. Barrett, P. Naumov

8:00 – 292. Planar arrays of artificial dipolar molecular rotors. P. Dron, J. Kaleta, E. Kaletová, A. Younes, G. Bastien, J. Wen, M. Cipolloni, M. Mašát, K. Zhao, Y. Shen, R. Shoemaker, T. Magnera, C. Rogers, **J. Michl***

8:30 – 293. Elasticity of crystalline molecular materials. **D. Hooks***, C. Bolme, K. Ramos, M. Cawkwell

9:00 – 294. Optically programmed buckling of polymer films and multilayers. **R. Hayward**

9:30 – 295. Programming mechanical adaptivity in liquid crystal polymer networks. **T.J. White**, T.H. Ware, V.P. Tonidiglia, J. Wie, M.E. McConney

10:00 – 296. What directs growth chirality of lamellar crystals of chiral polymers?. **J. Xu***, H. Ye, B. Guo

10:20 – 297. Optomechanical actuators for controlling mechanotransduction in living cells. **K. salaita**

10:40 – 298. Solar-powered nanomechanical molecular transduction in a crystalline rotor. **J. Cole**

11:00 – 299. Photonic effects in ruthe-nium sulfoxide polymers. **J. Rack**, M. Livshits

11:20 – 300. Mechanochromic luminescent difluoroboron beta-diketonate materials. T. Butler, W.A. Morris, C.A. DeRosa, M. Kolpaczynska, J. Samonina-Kosicka, A. Mathew, **C.L. Fraser**

Hawaii Convention Center
304A

Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157)

Organized by: S. Horikoshi, N. Serpone, R. Gupta, Y. Hayashi, M. Ashokkumar, M. Watana

Presiding: Y. Sakamoto, M. Sato, M. Watana

8:00 Opening remarks

8:05 Motoyasu Sato

8:05 – 301. Particle coating using the combination of plasma and spouted bed. **H. Sekiguchi***

8:30 – 302. Preparation of high quality CVD diamond using mode conversion type microwave plasma CVD. **Y. Sakamoto**

8:45 – 303. Chemical reaction induced by discharge plasma at pressurized argon/solution interface. **M. Goto***, Y. Hayashi, K. Mano, N. Takada, H. Kanda

9:00 – 304. Synthesis of carbon supported platinum catalyst produced by microwave induced plasma in liquid. **S. Sato***, H. Tsukamoto, K. Mori, O. Ariyada, T. Yonezawa

9:15 Yukihiko Sakamoto

9:15 – 305. Photodegradation of bromine-containing pollutants using microwave discharged electrodeless lamp (MDEL). **A. Tsuchida**, K. Oshima, S. Horikoshi

9:30 – 306. TiO₂: From nano to micro size for efficient photocatalysis applications. **E. Colombo**, M. Ashokkumar

9:45 – 307. Femtosecond photon sources and laser driven electron bunches based prethermal reaction processes. **Y. Gaudel***, C. Thaury, A. Doche, E. Chelnokov, V. Malka

10:00 – 308. Principal effects of high frequency piezoelectric fields on emerging chemical processing. **M. Sato***

10:15 Brack

10:30 Masaru Watana

10:30 – 309. Kinetics of the incorporation of metals for metalloporphyrin synthesis with inorganic metal salts in high temperature water. **T. Sato***, K. Ebisawa, K. Sue, S. Ito, T. Saito, N. Itoh

10:45 – 310. Generation of hydrothermal flames during supercritical water oxidation of organics. S.N. Reddy, **S. Nanda**, J.A. Kozinski*, M.C. Hicks, U.G. Hegde

11:00 – 311. Control of organic reactions in sub- and supercritical water using solid acid catalysts. **M. Akizuki***, Y. Oshima

11:15 – 312. Catalytic dehydrogenation of formic acid at mild temperature less than 100 °C under high pressure. **M. Iguchi**, Y. Manaka, Y. Himeida, H. Kawanami*

Hawaii Convention Center
Halls I, II, III

Electrochemistry on Boron-doped Diamond (BDD) Electrodes (#162)

Organized by: Y. Einaga, S. Park, O. Chaillapakul, J. Zhi, T. Kondo

Poster Session

10:00 – 12:00

313. Diamond synthesis on a centrifuge. **Y. Takagi***, Y. Inatomi, R. Nishimura

Hawaii Convention Center
319A

Natural to Nanosphere Lithographies: Two Decades of Self-assembled Advanced Materials (#177)

Organized by: A. Morfa, M. Giersig, K. Kempa, R. Duyne, L. Zhi
Presiding: E.M. Akinoglu

8:00 – 314. Colloidal crystal based soft lithography nanopatterning and its applications. **O. Park**

8:40 – 315. Latex particle templates guide evaporative lithography. **I. Valarelski***

9:00 – 316. Utilizing nanosphere lithography for the fabrication of nanopatterned aperiodic metal networks for transparent electrodes. **E.M. Akinoglu***, A. Morfa, M. Giersig

9:20 – 317. Copper mask nanosphere template lithography for broadly tunable plasmonic antennas. M. Swartz, M. Rodriguez, S. Blair, **J.S. Shumaker-Parry***

9:40 – 318. Self-optimizing and template-free growth of nanopatterned semiconductor light absorbers in response to spectral illumination. **A. Carim***, N. Batara, A. Premkumar, H. Atwater, N.S. Lewis

10:00 – 319. Self-assembled plasmonic structures. **G.C. Schatz***

10:40 – 320. Atomic layer deposition on heterogeneous nanostructured substrates. **C. Lancaster**, J.S. Shumaker-Parry

11:00 – 321. Home-built sample stage designed for force modulation microscopy using a tip-mounted AFM scanner. **J.C. Gorno**, L. Lu

11:20 – 322. Dual-assembled nanotemplates by PS-b-PMMA block copolymer lithography. **Y. Choi***, S. Kim

Hawaii Convention Center
320 Theatre

Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223)

Organized by: D. Jiang, W. Wang, W. Zhang

Presiding: R. Banerjee, T. Heine

8:00 – 323. From covalent organic frameworks over novel N_n-species to porous N-doped carbons: New porous materials by polymerization extending the usual range. **M. Antonietti***, N. Fechner, T. Fellinger, M. Shalom

8:25 – 324. Calculation of charge carrier mobility in covalent organic frameworks. **S. Irie***

8:50 – 325. Micropore engineering of carbonized porous aromatic framework (PAF-1) for supercapacitors. **T. Ben***, S. Qiu*

9:05 – 326. Metallated porous organic polymers: From hydrogen storage to electrocatalysis. **D. Liu***

9:20 Coffee Break

9:35 – 327. Surface confined 2D nanoporous networks: From supramolecular assembly to dynamic covalent chemistry. **D. Wang, I. Wan**

10:00 – 328. Development of functional porous organic polymers through dynamic covalent chemistry. **W. Zhang***, Y. Zhu, H. Yang, Y. Du, G. Lu, Y. Jin

10:25 – 329. Stacking, electronic and phonon confinement of layered covalent-organic frameworks and hybrid materials. **T. Heine***, P. Miro, M.A. Addicoat

10:50 – 330. Toward low-dimension porous nanomaterials through nanocarbon template-directed copolymerization. **F. Zhang***, X. Zhuang

11:05 – 331. Flowable nanospace in columnar liquid crystal. **K. Tanaka***, S. Kawano, M. Kata

11:20 – 332. Multifunctional organic frameworks for heterogeneous catalysis. **Y. Zhang**

Hawaii Convention Center
321A

Nanomaterials for Nanomedicine (#289)

Organized by: A. Maruyama, D. Lee, R. Narain
Presiding: H. Asanuma, X. Huang, J. Lee

8:00 – 333. Carbohydrate based nanomaterials for gene therapy. **R. Narain**

8:25 – 334. Stemless linear probe for the detection of RNA in living cell.

H. Asanuma*, M. Akahane, R. Niwa, Y. Kamiya, H. Kashida

8:50 – 335. Nanobio imaging of cancer metastasis with X-ray CT and fluorescence.

K. Gonda*, Y. Kubota, Y. Kobayashi, H. Higuchi, N. Ohuchi

9:05 – 336. Understanding endosomal escape using a pH responsive nanoparticle. **G.K. Such**, A.P. Johnston, S.K. Mann, A. Wong, E. Czuba

9:20 – 337. Advanced functional magnetic glyconanoparticles for disease detection. **X. Huang**

9:45 – 338. Noninvasive in-vivo imaging of neutrophil and tumor cells in mouse auricles. **H. Higuchi***

10:10 – 339. Intracellular pathways of peptide-conjugated quantum dots. **V. Biju**, S. Wakida, Y. Suzuki

10:25 Break

10:40 – 340. Engineered proteinoids for targeted cancer therapy. **J. Lee***

11:05 – 341. Nanopharmaceutical evaluation improved with aggregation-induced emission molecules. **X. Xue, C. Zhang, G. Zou, X. Liang***

11:30 – 342. Study on cellular responses of epidermal growth factor immobilized to gold nanoparticles. **J. Nakanishi***, S. Yamamoto, Y. Shimizu, K. Yamaguchi

11:45 – 343. Multifunctional polymeric nanoparticles for cancer imaging and therapy. **M. Wang**

Hawaii Convention Center
318B

Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308)

Organized by: R. Morandotti, D. Moss, F. Omenetto, N. Tsutsumi, K. Alamgir, K. Char, A. Facchetti
Presiding: N. Tsutsumi

8:00 – 344. Highly efficient dye sensitization of polymer solar cells. **H. Ohkita***, H. Xu, S. Honda, H. Benten, S. Ito

8:30 – 345. Polymers for optical technologies utilizing linear susceptibility. **S.Z. Cheng***

9:00 – 346. Toward the next level of electronics: From implantable to bioinspired devices. **T. Kim**

9:20 – 347. Mechanisms of metal deposition on colloidal gold nanoparticle substrates. **P.J. Straney**, J.E. Millstone*

9:40 – 348. Bench top fabrication of transferable micro/nanostructured gold electrodes for stretchable sensors and electronics. **Y. Zhu**, J. Moran-Mirabal*

10:00 Break

10:10 – 349. Organic solar cell interfacial science. **T.J. Marks**

10:40 – 350. High-efficiency multijunction polymer solar cells with PBDTTPD and wide-bandgap analogs. **P.M. Beaujuge***

11:00 – 351. Interfaces and nanostructures in organic solar cells. **K. Tajima**

11:20 – 352. Development and surface modification of highly impermeable, smooth, and transparent butyl rubber for stretchable electronics. **A. Vohra**, H. Filatratul, N. Suhan, C. Siegers, L. Ferrari, G.J. Davidson, T. Carmichael*

11:40 – 353. Approaches to solution processable n-channel π-conjugated donor-acceptor co-polymers and device applications. **Z. Yuan**, B. Fu*, Y. Jiang, M. Chang, P. Chu, D. Collard, E. Reichmanis*

Hawaii Convention Center
317B

Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery (#314)

Organized by: J. Schrier, C. Amador-Bedolla, S. Iwata, T. Woo
Presiding: C. Amador-Bedolla, S. Iwata, J. Schrier, T. Woo

8:00 Introductory Remarks

8:05 – 354. Machine learning for organic materials design. **A. Aspuru-Guzik***

8:45 – 355. Quantification of the structure-property relationship in polymeric semiconductors: An algorithmic, Big-Data approach. **N. Persson***, D. Nazarian, E. Reichmanis

9:15 – 356. Large-scale data-mining identifies new classes of dyes for dye-sensitized solar cells. **J. Cole**

* Principle Author

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9:45 Break

10:00 – 357. Chemoinformatic characterization of databases for drug discovery.
J.L. Medina-Franco*

10:30 – 358. Embedding parameters in ab initio theory to develop flexible models of electronic properties. **D.J. Yaron***, M. Tanha, H. Li, C.R. Collins, S. Kaul, A. Cappiello, G.J. Gordon

11:00 – 359. Machine learning for combinatorial materials science. **I. Takeuchi**

Hawaii Convention Center
316B

The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347)

Organized by: M. Srinivasarao, A. rey, H. Jung

8:00 – 360. Organizing principles of virus assembly. **M. Muthukumar***

8:35 – 361. How does white color vary in birds? **M. Shawkey***, B. Igic, L. D'Alba

9:10 – 362. Biological plywood structure characterisation method with "Aurigans Scarab" cuticle as example.

O. Aguilar Gutierrez*, A. Rey*

9:35 – 363. Structure and strength in collagen materials. **R.G. Haverkamp**, K.H. Sizeland, H.R. Kayed, H. Wells*, R.L. Edmonds, N. Kirby, A. Hawley, S. Mudie

10:00 Session Break

10:10 – 364. Specific interactions of multivalent carbohydrate surfaces mimicking the cells glyocalyx: Effect of mechanical flexibility, ligand density and molecular multivalency. H. Wang, S. Martin, F. Jacobi, T. Pompe, L. Hartmann, S. Schmidt

10:35 – 365. Modeling the physical structure and function of living biological soft matter. **M.G. Forest***

11:10 – 366. Phases and self-assembly of quasicrystalline lipid A-phosphate structures. **H.H. Paradies***

11:35 – 367. Molecular dynamics of π -conjugated polymers and application to bioinspired signal processing devices. **N. Asakawa***

Hawaii Convention Center
Halls I, II, III

Materials for the Mitigation of Chemical Hazards (#388)

Organized by: J. DeCoste, G. Peterson, J. Becker, M. Biggs, L. Croll, K. Walton
Presiding: J. DeCoste

Poster Session

10:00 – 12:00

368. Activated carbon-based gas sensors: Effects of surface features on the sensing mechanism. **N. Travlou**, M. Seredych, E. Rodriguez-Castellón, T.J. Bandosz

369. Poly(ethylene terephthalate) nanofiber sheet prepared by CO_2 laser supersonic continuous multidrawing. **A. Suzuki***, K. Hosoi, K. Miyagi

370. Amidoxime-based carbon-silica composite materials for carbon dioxide sorption. **P. Poudrel Ghimire**, C. Gunathilake, M. Jaroniec*

371. Zirconium (hydr)oxide/graphite oxide/AgNPs composites: Role of surface features in reactive adsorption of mustard gas and organophosphate surrogates' vapors. **D. Giannakoudakis**, T.J. Bandosz*

Hawaii Convention Center
314

Safety and Sustainability of Nanotechnology (#404)

Organized by: Y. Zuo, J. Ferri, C. Chen, J. Loo, S. Mylon
Presiding: Z. Liu, J. Loo, W. Parak, X. Shi

8:00 – 372. Quantification of nanoparticle uptake by cells and its correlation to basic physicochemical parameters.
W. Parak

8:30 – 373. Nanomaterials – exploiting their benefits, while enhancing their safety. **J. Loo**

8:55 – 374. Gd-metallocarbonerol nanomaterial $\text{Gd}@\text{C}_{60}(\text{OH})_{22}$ promotes activation of fibroblasts through up-regulating PDGF receptor protein levels. P. Wang, Y. Zhao, C. Chen*, Q.R. Miao*

9:20 – 375. "Biodegradable" metallic nanoparticle aggregates. **J. Berlin**

9:45 Coffee break

9:55 – 376. Nanotheranostics for imaging-guided cancer therapy: Fighting cancer metastasis. **Z. Liu***

10:20 – 377. Theranostic nanoprobes for breast cancers. **L. Zeng, Z. Shen**, W. Ren, J. Li, Z. Shi, X. Ma, L. Zhang, M. Zubair Iqbal, T. Chen, A. Wu*

10:45 – 378. Tunable rigidity of (polymeric core)-(lipid shell) nanoparticles for regulated cellular uptake. **X. Shi***, J. Sun, L. Zhang, J. Wang, X. Jiang

11:10 – 379. Application of mass production single-crystalline graphene quantum dots as antitumor drug carrier. **C. Li, L. Ding, C. Yao, P. Dong, M. Wu*, Y. Wang***

11:30 – 380. Synchrotron-based X-ray microscopic studies for bioeffects of nanomaterials. **Y. Zhu**, X. Cai, J. Zhang, Y. Zhang, L. Wang, C. Fan

Hawaii Convention Center
316C

Single-Molecule Function and Measurements (#408)

Organized by: T. Ogawa, H. Tada, S. Park, P. Weiss
Presiding: S. Park, J. Terao

8:00 Break

8:15 – 381. Synthesis and measurements of molecules bearing nonsymmetric single-molecule electric properties. **T. Ogawa***, M. Handayani, Z. Chen, N. Sakata, S. Lee, F. Miyamoto, T. Inose, R. Yamada, H. Tada, H. Tanaka

8:45 – 382. Molecular conductivity difference in isomeric polycyclic aromatic hydrocarbons. **H. Uno***, S. SATO, T. Tanimoto, M. Handayani, T. TAMAKI, M. Takase, S. Mori, T. Nakae, T. Ogawa

9:15 – 383. Structurally well-defined aminophenyl oligomers analogous to polyaniline: Synthesis, properties, and internal electron transfer. **K. YAMASHITA***, S. Takeuchi, K. SUGIURA*

9:35 – 384. Synthesis of insulated molecular wire and development of molecular wiring method by cross-coupling reaction. **J. Terao***

10:05 Break

10:20 – 385. Design, synthesis, and properties of novel units for single-molecular electronics. **Y. Ie***, R. Yamada, H. Tada, Y. Asa

10:40 – 386. Electronic properties of bottom-up synthesized graphene nanoribbons. **T. Nakae**, H. Sakaguchi*

11:00 – 387. Molecular alignment of mixed-valence dinuclear ruthenium complexes on single walled carbon nanotube. **H. Ozawa**, N. Katori, M. Haga

11:20 – 388. Self-aligned formation of sub 1 nm gaps utilizing electromigration during metal deposition. **Y. Naitoh***, r. matsushita, M. Mukaida, M. Kiguchi, K. Tsukagoshi, T. Ishida

Hawaii Convention Center
315

Advances in Organic Light-Emitting Diodes (#409)

Organized by: J. Bredas, C. Adachi, K. Wong, V. Yam, P. Burn, J. Kim
Presiding: J. Bredas

8:00 – 389. Efficient electroluminescence from heavy (Ir) and not so heavy (Cu) metal complexes. **M. Thompson***, R. Hamze, P. Saris, T. Batagoda

8:30 – 390. Development of materials and architectures for light-emitting diodes. **P.L. Burn***, R. Jansen-van Vuuren, F. Maasoumi, P. Meredith, E. Namdas

8:50 – 391. New trends in the design of transition-metal based OLED phosphors. **Y. Chi***

9:10 – 392. Phosphorus-based chromophores: Efficient emitters for OLEDs. **M. Hissler***

9:30 – 393. Different material concepts for the development of vapor and solution processable OLEDs. **T. Eberle***

10:00 BREAK

10:20 – 394. Vertical organic transistor for OLED driving. **H. Zan***, H. Meng

10:50 – 395. Highly efficient exciplex-based OLEDs. **K. Wong***

11:10 – 396. Microwave synthesis of tricyclometalated iridium complexes and their precise analysis by using a LC-TOF MASS method. **T. Matsumura***, N. Shimizu, H. SAWADA, J. Kido, H. Sasabe

11:30 – 397. RISC from high-lying triplet to singlet: Optical probes and application for OLEDs. **Y. Ma***, B. Yang, D. Hu, L. Yao

Hawaii Convention Center
319B

Self-assembled Biofunctional Nanomaterials (#433)

Organized by: R. Nagarajan, K. Sakurai, H. Chen

8:00 – 398. Shape persistence micelles having the same aggregations with the platonic solids. **K. Sakurai**

8:20 – 399. Self-assembly of lipid-polymer nanodiscs for membrane protein supports. **K. Edler***, I. Idini, C. Tognoni, T. Dafford, S. Lee, A. Terry, T. Arnold, D. Barlow, J. Curtis

8:50 – 400. Hydrophobe-uptake micellization of low molar mass and polymer surfactants in aqueous media. **K. Morishima, T. Sato***

9:20 – 401. Entropically-induced phase transition for strongly confined semi-flexible polymers. **Y. Chen**, D. Luzhbin, G. Liao

9:50 Break

10:00 – 402. Molecular mechanism of surface-assisted self-assembly of amyloid-like peptides. **S. Kang***, T. Huynh, R. Zhou

10:20 – 403. Structure of DNA-dendrimer complexes and its implication on DNA-histone interaction in nucleosome. **H. Chen**

10:50 – 404. Stability of aqueous biofilms of the Class II hydrophobin Cerato-ulmin in the presence of gaseous and liquid hydrocarbons: A phenomenological investigation. **X. Zhang**, P.S. Russo, B. Blalock, w. huberty

11:10 – 405. Small-angle scattering of anisotropic nanoparticles and their assemblies. **A.J. Senesi**, B. Lee*

11:30 – 406. Nanostructure and stimuli-responsibility of poly(betaine) brushes at the air/water interface. **H. Matsuoka***, A. Sakamoto, Y. Mochizuki

Wednesday Afternoon

Hawaii Convention Center
318A

Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95)

Organized by: J. Kawamata, J. Choy, C. Detellier, H. Zhang, J. Huang, L. Wan
Presiding: J. Kawamata, T. Nakato

13:00 Opening remark

13:05 – 407. Synthesis, properties, and applications of Group IV graphane analogs. **J. Goldberger***

13:30 – 408. New strategy for the construction of 2D monolayer. **X. Hou**, C. Ke, J.F. Stoddart*

13:50 – 409. Aerogels based on 2D nanosheets: Graphene, boron nitride, and beyond. **M.A. Worsley***

14:10 – 410. 2D nanosheet architectonics for tailored electronics. **M. Osada***, T. Sasaki

14:30 – 411. Atomtronics: The application of organometallic bis-hexahapto bonding to the electrical interconnection and electronic conjugation of the graphitic surfaces of carbon nanotubes and graphene. **R.C. Haddon**

15:00 Break

15:10 – 412. Crystalline hybrid structures built on semiconductor nanomodules designer materials for general lighting applications. **J. Li***

15:35 – 413. Carbon nanomembranes (CNMs) from molecular monolayers. **A. Goelzhaeuser***

15:55 – 414. Biomass-directed mass production of h-BN nanosheets for highly thermoconductive polymeric composites. **X. Jiang***, X. Wang*

16:15 – 415. Expanding the range of applications of AlN through its scalability at the 2D limit. **R. dos Santos, R. Rivelino, F. de Brito Mota, A. Kakanakova-Georgieva, G. Guerouiev***

16:35 – 416. Functional 2D crystals: Controlled synthesis and optoelectronic devices. **H. Peng**

Hawaii Convention Center
317A

Design, Synthesis and Applications of Advanced Porous Materials (#111)

Organized by: C. Doonan, M. Dinca, S. Telfer, S. Furukawa, Q. Li

13:00 – 417. Framework dynamics: extreme thermomechanical behaviours through a porous molecular materials approach. **C. Kepert***

13:30 – 418. Metal-organic frameworks with dynamic interlocked components. **K. Zhu, V.N. Kukotic, C. O'Keefe, R. Schurko, S. Loeb***

14:00 – 419. Metal-organic frameworks toward gas biology applications. **S. Furukawa***

14:20 – 420. Near-infrared emitting metal-organic frameworks for biological imaging applications. **N. Rosi**, S. Petoud, C. Liu, K. Gogick, A. Foucault-Collet, S. Villette

14:40 – 421. Engineering metal-organic frameworks. **P. Falcaro***

15:00 – 422. Fast triplet exciton diffusion in metal-organic frameworks for ultralow power photon upconversion. **N. Yanai***, P. Mahato, N. Kimizuka

15:15 – 423. MOFs for use in mixed matrix membranes, produced at scale. **M.R. Hill**

15:30 – 424. Mimicking geological mineralization for the synthesis of porous materials in the solid state. **C. Mottillo**, Y. Lu, P. Minh-Hao, T. Do, T. Friscic

15:45 – 425. Structural diversity of SURGELS for bio-application. **S.K. Schmitt***, M. Tsotslas, S. Diring, S. Furukawa, H. Gleemann, S. Kitagawa, C. Woell

16:00 – 426. 3D superstructures of metal-organic frameworks synthesized via coordination replication. **K. Sumida***

16:15 – 427. Iodine adsorption in ZIF-8 and related structure: A computational investigation. **B. Chang***, P.D. Bristowe, A.K. Cheetham

* Principle Author

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16:30 – 428. Biomimetically mineralized metal-organic frameworks and its potential in biotechnology. **K. Liang**, P. Falcaro, C. Doonan

Hawaii Convention Center
316A

Frontier and Perspectives in Molecular Spintronics (#127)

Organized by: M. Yamashita, B. Zhang, H. Tajima, B. Hu, P. Lahti, J. Gao
Presiding: H. Tajima, M. Yamashita

13:00 – 429. Organic spin-valve based upon the spin state manipulation of paramagnetic tris(8-hydroxyquinoline)iron(III) molecules. **D. Sun***, Z. Vardeny*

13:30 – 430. Carbon electrode-molecule junctions: A reliable platform for molecular electronics. **x. guo**

14:00 – 431. Carbon nanotube based field-effect transistors: Merits and fundamental limits. **L. Peng***

14:30 – 432. Interface-assisted molecular spintronics. **K.V. RAMAN***

15:00 Break

15:15 – 433. Metal-radical materials for tunable spin physics. M. Vaz, M.A. Novak, H. Akpinar, R.A. Cassaro, **P.M. Lahti***

15:45 – 434. Magneto-optical properties in organic-inorganic perovskites. **B. Hu***

16:15 – 435. Photo-CELIV experiments under magnetic field. **H. Tajima***

Hawaii Convention Center
321B

Applications of Ultrasound to Nanoscience (#150)

Organized by: K. Suslick, F. Grieser, M. Atobe, J. Yu, S. Jeong
Presiding: M. Atobe, K. Suslick

13:00 – 436. Temperature non-equilibration during single-bubble sonoluminescence. **D.J. Flannigan***, K.S. Suslick*

13:30 – 437. Influence of short frequency ranges on cavitation activity in HIFU sonoreactors. J.T. Lee, L. Hallez, **J. Hihn**, F. Touyeras, A. Nevers, M. Ashokkumar

14:00 – 438. Continuous industrial-scale processing of liquids by high-amplitude ultrasound. **A.S. Peshkovsky***

14:20 Coffee & Bio Break

14:30 – 439. Application of ultrasound to the formation of amino acids from prebiotic gases. **F. Grieser***, L. Dharmarathne

15:00 – 440. Effects of various parameters on sonochemical degradation of aromatic compounds in water. **K. Okitsu**

15:30 – 441. Determining the mechanism of ultrasonic activation of persulfate. Z. Wei, F.A. Villanueva, **L. Weavers**

16:00 – 442. Hot spots in solids created with an ultrasonic hammer. **K. Suslick**, D. Dlott, M. Chen, S. You

Hawaii Convention Center
322AB

Mechanically Responsive Materials (#153)

Organized by: P. Naumov, T. White, B. Kahr, Y. Yu
Presiding: J. Rack, T.J. White

13:00 – 443. Photoinduced bending, twisting, and grabbing in anthracene-based microcavats. **C. Bardeen***, R. Al-Kaysi, f. tong, t. kim, l. zhu, l. mueller, c. yang

13:30 – 444. Opto-mechanical azo materials: New light on mechanism and optimization. **C. Barrett***, O. Bushuyev, T. Friscic

14:00 – 445. Chemomechanoresponsive systems mimicking natural mechano-transduction processes. **P. SCHAAF***

14:20 – 446. Quantification, systematics, and modeling of mechanical effects in molecular crystals. **P. Naumov***

14:40 – 447. Light-induced crawling of crystals of azobenzene derivatives on a glass surface. **Y. Norikane**

15:00 – 448. Photodeformable liquid crystal polymers and bioinspired applications. **Y. Yu***, J. Lv, Y. Liu

15:20 – 449. Stimuli-responsive polymer materials. **A. Schenning**

15:40 – 450. Multiple stimuli responsiveness of spiropyran-incorporating nanoporous frameworks. **R. Klajn***, P. Kundu

16:00 – 451. Mechano and light responsive polymer composites and conducting polymers. **M. Schulz-Sentf**, S. Sindushree, R. Adelung, A. Staubitz*

16:20 – 452. Elastic flexibility in molecular crystals of metal complexes. **A. Worthy***, M. Pfirrmann, A. Grosjean, J. Clegg, J. McMurtie

16:40 – 453. Mechanical analysis of soft materials by a surface labeled grating method. **A. Shishido**

Hawaii Convention Center
304A

Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157)

Organized by: S. Horikoshi, N. Serpone, R. Gupta, Y. Hayashi, M. Ashokkumar, M. Watanabe

Presiding: R. Gupta, A.T. Quitain, T. Sato

13:00 Ram Gupta

13:00 – 454. Hydrothermal reduction of CO₂ to formic acid with general Fe powder. **J. Du***, L. Lyu, G. Yao, Z. Huo, F. Jin*

13:15 – 455. Gasification characteristics of arginine in supercritical water conditions. **T. Samamulya**, Y. Matsumura*

13:30 – 456. Catalyzed supercritical water gasification of sewage sludge using a bench-scale flow reactor. **O. Sawai***, T. Nunoura

13:45 – 457. Fabrication of chalcogenide semiconductor films using supercritical ethanol dissolving low-cost solid chalcogen sources. **T. Tomai***, Y. Nakayasu, I. Honma

14:00 – 458. Biodiesel production in supercritical methyl acetate: experimental investigation and kinetic model.

O. Farobie, Y. Matsumura*

14:15 – 459. Reactive separation employing the synergy of mixed subcritical H₂O/supercritical CO₂ system. **A.T. Quitain***, T. Takayama, M. Sasaki, T. Kida

14:30 – 460. Kinetics of hydrothermal separation of lignin and characteristics of the lignin. **M. Watanabe***, Y. Kanguri, T.M. Aida, R.L. Smith

14:45 – 461. Catalytic conversion of limonene in supercritical carbon dioxide media. **M. Aomatsu***, A.T. Quitain, T. Kida, M. Sasaki, M. Tanaka, M. Hosino

15:00 Brack

15:15 Armando Quitain

15:15 – 462. Inhibition of char deposition using a particle bed in heating section of supercritical water gasification. **S. Hirota**, S. Inoue, T. Inoue, Y. Kawai, Y. Wada, T. Noguchi, Y. Matsumura*

15:30 – 463. Role of organic acids as intermediates of xylose decomposition in sub- and supercritical water. Y. Matsumura*, N. Pak Sung, R. Nagano

Hawaii Convention Center
320 Theatre

Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223)

Organized by: D. Jiang, W. Wang, W. Zhang

Presiding: L. Chi, N. McKeown

13:00 – 464. Photo-induced charge transfer in covalent organic frameworks. **T. Bein***

13:25 – 465. Conjugated porous organic polymers for gas sorption and separation. **B. Han***

13:50 – 466. 2D molecular covalent networks via surface-assisted reactions. **B. Yang, X. Shen, Q. Li, L. Chi**

14:15 – 467. Breakthrough reusable and porous β -cyclodextrin sorbent for instant water purification. **A. Alsabae***, B. Smith, L. Xiao, W. Dichtel

14:30 – 468. Micro vs. macrofluidics: Encapsulation of hydrochloric acid in porous polymer beads. **J. Ferrer***, A. Menner, A. Bismarck

14:45 Coffee Break

15:00 – 469. Porous liquids based on hollow nanostructures. **S. Dai**

15:25 – 470. Fullerene-stabilised phthalocyanine nanoporous crystals. **N. McKeown***, C.G. Bezzu, L. Burt, S. Moggach, B. Karuchi

15:50 – 471. Supramolecular organic framework: periodic self-assembled structures in water. **Z. Li**

16:15 – 472. Highly microporous free-radically generated polymeric materials using a novel contorted monomer. **M. Wendland***

16:30 – 473. Multifunctional applications of porous covalent-organic materials. **D. Caو**

16:45 – 474. Peptide-MOF chemical motors that sense PbSe nanoparticles. **Y. Ikezoe***, J. Fang, T.L. Wasik, M. Shi, T. Uemura, S. Kitagawa, H. Matsui

Hawaii Convention Center
321A

Nanomaterials for Nanomedicine (#289)

Organized by: A. Maruyama, D. Lee, R. Narain

Presiding: z. Gu, K. Ishihara, M. Winnik

13:00 – 475. Novel polysaccharide carrier for functional oligonucleotides: Immunocyte targeting drug delivery system. **K. Sakurai***, S. Mochizuki

13:25 – 476. Bioinspired design of dynamic macromolecular for gene delivery. **z. Gu***

13:50 – 477. Conformational changes of DNA monitored by fluorescence blinking. **K. Kawai***, A. Maruyama, T. Majima

14:05 – 478. DNA origami nanopores: An emerging tool in bionanotechnology. **S.M. Hernandez Ainsa***, K. Göpfrich, U. Keyser

14:20 Break

14:35 – 479. Hybrid exosomes for new drug delivery system. **K. Akiyoshi***

15:00 – 480. Metal chelating polymer-based radioimmunoconjugates for tumor imaging and cancer therapy. **M. Winnik***, Y. Lu, P. Liu, A.J. Boyle, G. Ngo Djock Mbong, R.M. Reilly

15:25 – 481. Photosensitizing peptides and proteins for photochemical internalization. **T. Ohtsuki***, S. Miki, H. Fujiwara, M. Kitamatsu, K. Hirakawa, S. Okazaki, K. Watanabe

15:40 break

15:50 – 482. Self-assembled nano aggregates based on amphiphilic polyaspartamide graft copolymers: Intracellular uptake and pH dependent drug release. **D. Kim**

16:15 – 483. Cyocompatible polymeric nanoparticles for delivery of biomolecules into cells. **K. Ishihara***

16:40 closing remark

Hawaii Convention Center
318B

Advanced Materials for Photonics and Electronics: Recognizing the Research of Tobin J. Marks (#308)

Organized by: R. Morandotti, D. Moss, F. Omenetto, N. Tsutsui, K. Alamgir, K. Char, A. Faccetti

Presiding: A. Faccetti

13:00 Introductory Remarks

13:05 – 484. Nature inspired conjugated small molecules and polymers as next generation semiconductors.

M. Al-Hashimi*, H. Bronstein*, H.S. Bazzi*, D. Seapy*, T.J. Marks*

13:20 – 485. Stretchable electronics. **Z. Bao***

13:35 – 486. Pyridine coordination chemistry for molecular assemblies. **M.E. van der Boom***

13:50 – 487. Recent fused-thiophenes-based small molecules development for organic thin film transistors (OTFTs). **M. Chen***

14:05 – 488. Theory guided design of nano-photonics electro-optic materials and devices. **L.R. Dalton***

14:20 – 489. Printing circuits. **D. Frisbie**

14:35 – 490. Materials design for high-performance organic thin-film transistors and polymer solar cells. **X. Guo**

14:50 Break

15:00 – 491. Solution processing and device integration at the 2D limit. **M.C. Hersam***

15:15 – 492. Charge carrier injection into molecular crystals at the contact interfaces. **T. Inabe***

15:30 – 493. Inorganic-organic hybrid perovskites: Chemistry and solar cells. **M. Kanatzidis***

15:45 – 494. Getting new tools for a more sustainable organic electronics. **A. Marrochini***

16:00 – 495. Materials for soft, bioreversible optoelectronic interfaces to the brain. **J. Rogers**

16:15 – 496. Stimuli-eresponsive imide-based π -conjugated systems: Structural dynamics and electronic properties. **A. Takai, M. Takeuchi**

16:30 – 497. Aggregation and morphology control enables multiple cases of polymer solar cells with efficiencies near 11%. **H. Yan**

16:45 – 498. Low-temperature sol-gel metal oxide-based flexible electronics. **M. Yoon**

Hawaii Convention Center
317B

Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery (#314)

Organized by: J. Schrier, C. Amador-Bedolla, S. Iwata, T. Woo
Presiding: C. Amador-Bedolla, S. Iwata, J. Schrier, T. Woo

13:00 Introductory Remarks

13:05 – 499. Developing properties databases for functional materials and devices: A first step towards machine learning. **R. Seshadri**

13:35 – 500. Dark reactions project: A machine learning approach to materials discovery. **A. Norquist**

14:05 – 501. High-throughput ab initio study for 2D electrode materials. **T. Tada**, T. Inoshita, H. Hosono*

14:35 – 502. Ferroic materials discovery guided by Bayesian principles. **J. Rondinelli**

15:05 Break

15:20 – 503. Accelerating materials research through machine learning. **T. Mueller***

15:50 – 504. Discovery of nanoporous materials for energy application. **M. Haranczyk***, C. Simon, R.L. Martin, B. Smit

16:20 – 505. Enabling applications of nanoporous materials using first-principles-based screening. **D. Sholl***, D. Nazarian, J. Camp, R. Awati, S. Nair

* Principle Author

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Hawaii Convention Center
314

Safety and Sustainability of Nanotechnology (#404)

Organized by: Y. Zuo, J. Ferri, C. Chen, J. Loo, S. Mylon
Presiding: J.K. Ferri, H. Galla, S. Mylon, Y. Zuo

13:00 – 506. Interaction of nanoparticles with lipid monolayers and lung surfactant films. **H. Galla***

13:30 – 507. Biophysicochemical interactions between nanoparticles and pulmonary surfactants. **Y. Zuo***

13:50 – 508. Toxicity of nanofilm spray products. The role of lung surfactant function. **S. Larsen***, J.B. Sorli, A.W. Norgaard, Y. Huang, J.S. Hansen

14:10 – 509. Interaction between inhaled graphene oxide nanosheet and pulmonary surfactant monolayer. **G. Hu**, Q. Hu, Y. Zuo

14:30 Coffee break

14:40 – 510. Effects of polymer-coated nanoparticles on the phagocytic capacity and viability of immune cells. **G.G. Goss**, V. Ortega, S. Memon, L. Unsworth, J. Stafford

15:10 – 511. Transformation and hazard potential of copper particles in a septic system using a zebrafish high-throughput screening assay. A.A. Taylor, **S.L. Walker**

15:35 – 512. Fine control of aggregation state of biocompatible polymer functionalized nanoparticles: Theory and experiment. F. Gambinossi, M. Chanana, **S. Mylon***, J.K. Ferri*

16:00 – 513. Interactions of chemical mechanical planarization nanoparticles with model biological membranes. **X. Liu**, K. Chen

Hawaii Convention Center
316C

Single-Molecule Function and Measurements (#408)

Organized by: T. Ogawa, H. Tada, S. Park, P. Weiss
Presiding: T. Ogawa, H. Uno

13:00 – 514. Spin properties of adsorbed magnetic molecule detected by Kondo feature. **T. Komeda***, T. Inose, D. Tanaka, T. Ogawa, F. Wu, Z. Shen

13:30 – 515. Control of single molecular conductance with STM atom manipulation. **T.K. Yamada***, N.K. Nazriq, S. Nakashima, N. Ohta

13:50 – 516. Molecular nanomagnets on graphene: A path towards hybrid molecular spintronics devices. **M. Affronte***

14:10 – 517. Theoretical study of a contact-asymmetry effect on magnetoresistance of single molecular spin valves. **T. Ohto***, R. Yamada, H. Tada

14:30 Break

14:45 – 518. Is "luminescent molecular pixel" feasible? Frustrating intermolecular energy transfer in the condensed state. **S. Park***

15:15 – 519. Single molecule control of adhesion and friction by cyclodextrins. **G. Wenz***, M. Albrecht, R. Bennewitz, J. Blas, B. Bozna

15:35 – 520. Carbon nanomaterials-based single-molecule electrical biosensors. **X. guo**

Hawaii Convention Center
315

Advances in Organic Light-Emitting Diodes (#409)

Organized by: J. Bredas, C. Adachi, K. Wong, V. Yam, P. Burn, J. Kim
Presiding: K. Wong

13:30 – 521. Controlling and imaging self-assembly for optoelectronic devices. **L. De Cola**, A. Aliprandi, A. Ruiz Carretero, M. Mauro

14:00 – 522. Emitting dipole orientation of phosphorescent dyes in OLEDs. **J. Kim***, C. Moon, K. Kim, J. Lee

14:20 – 523. Magnetic modulation of the light emission in a spin-OLED. J. Prieto-Ruiz, H. Prima-Garcia, A. Riminiucci, P. Graziosi, **V.A. DEDIU***, E. Coronado

14:40 – 524. Exciton migration in organic materials with enhanced optical effects. **t. goodson***

15:00 – 525. Novel core chromophores based on specific chemical structures and their effects. J. Lee, S. Kim, H. Shin, H. Lee, H. Jung, **J. Park***

15:30 Break

15:50 – 526. Organic light-emitting diodes: Approaches to facilitating charge-carrier injection and for efficient emissive layers. S. Barlow, D. Cai, C. Fuentes-Hernandez, M.P. Gaj, A.J. Giordano, W. Haske, X. He, D. Kang, T.M. Khan, B. Kippelen, **S.R. Marder***, K. Moudgil, S. Paniagua, F. Pulvirenti, S. Zhang, Y. Zhang, C. Zuniga

16:20 – 527. Molecular design of metal-free purely organic phosphors. **J. Kim***, M. Kwon, J. Jung, D. Lee, O. Bolton

16:40 – 528. Novel approaches to improve charge balance and light management in solution-processed phosphorescent OLEDs. **N. Stigelin**

17:00 – 529. In situ investigations of the solution-to-solid phase transformation of organic semiconductors. **A. Amassian**

Hawaii Convention Center

319B

Self-assembled Biofunctional Nanomaterials (#433)

Organized by: R. Nagarajan, K. Sakurai, H. Chen

13:00 – 530. Small angle X-ray scattering from polydop-shaped DNAs and their activity of cytokine secretion. **Y. Sanada**, T. Shiomi, T. Okobira, M. Nishikawa, Y. Takakura, K. Sakurai

13:30 – 531. Modeling of synthesis of well-defined nanoparticles and nanostructures. **V. Privman***

13:40 – 532. Interpolyelectrolyte nanoassembly to engineer DNA, peptides, and lipids. **A. Maruyama***

14:10 – 533. Exploration of spatial distribution of drug molecules incorporated in polymer micelles with anomalous small-angle X-ray scattering. **I. Akiba***, R. Nakanishi, K. Sakurai

14:30 – 534. Nanoscale protein-polymer interactions and potential contributions to solid-state nanobioarrays. **J. Hahn***

15:00 Break

15:10 – 535. Supramolecular nanoassemblies responsive to biological stimuli. **S. Thayumanavan**

15:40 – 536. Characterization of micelles formed from a model pluronic F127-BSA conjugate. **E. Hirst**, R. Nagarajan

16:00 – 537. Micelle structure and interactions in aqueous solutions: Modulation by polymers, cosolvents, and solutes. **A.I. Fajalia, P. Alexandridis, M. Tsianou***

16:20 – 538. Structural characteristics of DNA-Poly(N-isopropylacrylamide) bioconjugate. **M. Fujita**, M. Maeda

16:40 – 539. Dimerization of the type IV pilin from *Pseudomonas aeruginosa* strain K122-4 and its oligomerization into protein nanotubes. **G.F. Audette***, C. Lento

Wednesday Evening

Hawaii Convention Center
318B

Nanocrystal Synthesis, Characterization, Assembly and Applications (#34)

Organized by: R. Tilley, S. Skrabalak, T. Hyeon, T. Nann, T. Adshiri

19:00 – 540. Synthesis and growth mechanism of high-aspect-ratio gold nanorods in a gelled surfactant solution. **Y. Takenaka***, Y. Kawabata, H. Kitahata, M. Yoshida, Y. Matsuzawa, T. Ohzono, N. Yamada, H. Seto

19:15 – 541. From bare metals to metal oxides nanoparticles and hierarchical supramolecular metal oxide nanoparticle network assemblies. **E. Redel**

19:30 – 542. Pasmonic consequences of symmetry breaking in DNA-assembled 1D nanoparticle superlattices. **M.R. Jones**, M. O'Brien, K. Holstedt, G.C. Schatz, C.A. Mirkin

19:45 – 543. Study of AuFePt ternary alloy nanoparticles as a functional hybrid magneto-plasmonic system. **P. Mohan**, M. Takahashi, K. Higashimine, D. Mott, S. Maenosono*

20:00 – 544. Highly luminescent and transparent silica aerogels containing silicon nanocrystals. **M. Aghajamali***, M. Iqbal, L. Hadidi, T.K. Purkait, J. Veinot

20:15 – 545. Multifunctional engineered nanomaterials: Synthesis, fundamentals, and applications. **S.E. Hunyadi Murph**

Hawaii Convention Center
Halls I, II, III

Conjugated Polymers for Biological Applications (#43)

Organized by: H. Yu, S. Wang, J. Tovar
Presiding: S. Luo, J.D. Tovar, S. Wang, H. Yu

Poster Session

19:00 – 21:00

546. Development of novel polymeric prodrugs synthesized by mechanochemical solid-state polymerization of polysaccharides and vinyl monomers. **N. Doi**, Y. Sasai, Y. Yamauchi, M. Kuzuya, S. Kondo*

547. Synthesis and characterization of cationic polythiophene derivatives (II): DNA sensing. **T. Ishiyama**, Y. Erika, M. Fujita, Y. Takeoka, M. Hikukawa

548. Compendium method for surface modification with zwitterionic polymers and application to biomaterial development. **M. Nishida**, T. Nakaji-Hirabayashi, H. Kitano*

549. Construction of thin gel layer on the material interface using polymer brush and interpenetrating polymer network. **Y. Yamazawa**, T. Nakaji-Hirabayashi, H. Kitano*

550. Development of 2-nitrobenzyl-type photodegradable linker having the various substituent groups in benzyl position and fabrication of photoresponsive substrate towards cell patterning. **H. Ikegami**, J. Nakanishi, K. Yamaguchi

551. Control of conjugated polymer nanoparticle size and emission properties through microfluidics synthesis. **T.F. Abellha***, T.W. Phillips, J.C. de Mello, M.A. Green, L. Dailey

552. Optimization of the formulation of photoluminescent conjugated polymer nanoparticles for diagnostics and bioimaging. **L. Urbano***, H. Ku, K. Vanderla, T.F. Abellha, T. Desai, R. Harvey, M.A. Green, L. Dailey

553. Visual biomolecular detection based on dual polymerization-assisted amplification. **J. Yang**

554. Application of photothermal conducting polymer for harvesting of cell sheets. **M. Han**, J. Na, J. Kim, E. Kim*

555. Fabrication of natural material coated on the biodegradable fiber with calcium carbonate for improving hemostatic effect. **J. PARK**, K. Kyung, S. Kim, S. Shiratori*

556. Antimicrobial application of bioluminescence resonance energy transfer (BRET) system. **H. Bai***

Hawaii Convention Center
Halls I, II, III

Molecular Adsorption on Metallic Interfaces: Beyond the Cartoons (#102)

Organized by: D. Bizzotto, I. Burgess, H. Yu, T. Sagara, H. Yang

Poster Session

19:00 – 21:00

557. Quantitative analysis of thiolated ligand exchange on gold nanoparticles monitored by ¹H NMR spectroscopy. **A.M. Smith***, K.A. Johnston, L. Marbella, J.E. Millstone

558. Probing plasma protein binding to Au/Ag nanoparticles using FT-IR spectroscopy. **S. Yu**, M. Wang, **C. Fu**

559. Adsorption of cations on gold electrode surface investigated by ATR-SEIRA spectroscopy. **M. Futamata***, F. Watanabe

Hawaii Convention Center
Halls I, II, III

Design, Synthesis and Applications of Advanced Porous Materials (#111)

Organized by: C. Doonan, M. Dinca, S. Telfer, S. Furukawa, Q. Li

Poster Session

19:00 – 21:00

560. Vapochromic luminescence coupled with drastic change of ion-conductivity of ruthenium(II)-metalloligand-based porous coordination polymer. **w. ayako**, A. Kobayashi*, M. Yoshida, M. Kato*

561. Preparation of hollow silica spheres with mesopores using hybrid organic templates method. **H. Shibata**, H. Endo, T. Ogura, K. Hashimoto

562. Flexible solid-state supercapacitor based on a metal-organic framework interwoven by electrochemically-deposited PANI. **L. Wang**, X. Feng, B. Wang*

563. Synthesis of HEU-type zeolites and its application for steam reforming of dimethyl ether. **S. Watabe**, N. Shimoda, S. Satokawa*

564. Preparation of porous solids by acid-treatment of silica-pillared fluorine micas. **T. Yamaguchi**, Y. Soda, S. Taruta

565. Regulation of NO uptake in flexible paddlewheel-type Ru dimer chains with highly electron-donating dopants. **J. Zhang***, W. Kosaka, Y. Sekine, K. Taniguchi, H. Miyasaka

566. Photoinduced postsynthetic polymerization of a metal-organic framework toward a flexible stand-alone membrane. **Y. Zhang***, X. Feng*, H. Li, B. Wang*

567. Water-stable metal-organic framework for CO₂ capture. **R. Zhong***, X. Huang

568. Fluorescent chromophore encapsulated in porous metal-organic frameworks with tunable emission. **M. Song***, D. Yan

569. Carbon dioxide adsorption of MOF-74@PS with high water stability. **H. Kim***, J. Moon, D. Chun, Y. Park

570. Dual stimuli-responsive smart membrane for multiple on-off gates. **B. Lee**, S. Hyun, J. Kim*

571. Metal-organic framework-assisted synthesis of high efficient alcohol oxidation catalyst. B. Kim, H. Kim, **C. Lee***

* Principle Author

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572. Novel MV-templated zinc gallophosphate zeolite with dual photo-/thermochromism and tunable photo voltaic activity. **J. Li**

573. Metal-organic frameworks with both [2]rotaxane and porphyrin components: Toward the control of dynamics in solid state materials. **P. Martinez-Bult***, K. Zhu, S. Loeb

574. Room temperature phosphorescence from Coronene@ZIF-8. **H. Mieno***, R. Kabe, N. Notsuka, C. Adachi

575. Periodic mesoporous boron nitride at high pressure. M. Mandal, C. Liu, Y. Fei, **K. Landskron***

576. Supramolecular assembly of metal organic nanotubes with unique water transport properties. **T.Z. Forbes**

577. Preparation of Pt-included hollow silica and its activity for CO oxidation. **T. Mori***, N. Ikemaga

578. Porous polymer materials by reactive gelation: From preparation to applications. A. Bultzung, A. Cingolani, H. Wu, **G. Storti**, M. Morbidelli*

579. Electrochemical approaches for precise structural and property control: Porous nanomaterials for energy and environmental applications. **Y. Li***

580. NanoFoams: High purity transition metal, lanthanide nitride, and actinide oxide foams prepared from nitrogen-rich metal precursors. **J.M. Veauthier***, B.C. Tappan, D.E. Chavez, J.L. Kiplinger, K.P. Browne, N. Travia

581. Organic radicals installed metal-organic frameworks. **G. Ning**, K.P. Loh*

582. Chiral dopants and tropos ligands: Toward functional chiral periodic mesoporous organosilica (PMO) materials. **L.M. Reid**, C. Cruden*

583. Enhancement of porosity in NbO type metal-organic framework by post-synthetic reductive elimination. **T. Okamura**, S. Takaiishi, M. Yamashita*

584. Designed synthesis of large-pore crystalline polyimide covalent organic frameworks. **Q. Fang**, Y. Yan, S. Qiu

585. Synthesis of Fe@C core-shell particle and its applications in water treatment. **Q. Huo**, X. Li, L. Zhang

586. Conformationally flexible metal-organic framework. **R.B. Amador**, N. Godinez, C. Gutierrez*

587. Controlling microtube/microrod crystal morphology of metal-organic hexagons with a nanotubular supramolecular packing. **X. Cheng***, X. Chen

588. Synthesis and sorption properties of hollow porous carbon spheres made from a simple pyrolysis of core-shell type metal-organic framework (MOF). **S. Choi***, H. Lee, M. Oh*

589. In situ observation of a reversible Michael adduct by the crystalline sponge method. **V. Duplan**, H. Sato, M. Hoshino, Y. Inokuma, L. Wei, T. Honda, M. Fujita*

Hawaii Convention Center
Halls I, II, III

Frontier and Perspectives in Molecular Spintronics (#127)

Organized by: M. Yamashita, B. Zhang, H. Tajima, B. Hu, P. Lahti, J. Gao

Poster Session 19:00 – 21:00

590. Photostability enhancement of pentacene derivative by introducing radical substituent. **A. Shimizu***, A. Ito, Y. Teki

591. Organic thin film devices of TFT-metal complexes with paramagnetic Cu(II) ion. **A. Wachi**, H. Nishikawa*, M. Chikamatsu, R. AZUMI

592. Giant negative magnetoresistance effect in a molecular conductor based on iron(III) tetrabenzoporphyrin. **M. Nishi**, M. Matsuda, M. Ikeda, N. Hanasaki, N. Hoshino, T. Akutagawa

593. Organic electroluminescent devices consisting of dye-doped spin crossover complex films. **M. Matsuda**

Hawaii Convention Center
322AB

Mechanically Responsive Materials (#153)

Organized by: P. Naumov, T. White, B. Kahr, Y. Yu
Presiding: C. Bardeen, Y. Yu

19:00 – 594. Understanding mechanically reconfigurable organic single crystals. **C. Malli Reddy**

19:20 – 595. Photosalient behavior of crystals during [2+2] cycloaddition reactions. **J.J. VITALL***, R. Medishetty, P. Naumov

19:40 – 596. Photosalient effect of gold(II) complex through strengthening metallophilic interactions. **T. Seki**, H. Ito

20:00 – 597. Smart optical windows: Reversibly switching between high transparency, color display, and opaqueness. **S. Yang***

20:20 – 598. Photomechanical motion of crystals. **H. Koshiba***

20:40 – 599. Generalized high-accuracy universal polarimeter study on chiral salicylidenephenylethyamine crystals showing photomechanical effect. **T. ASAHI***

Hawaii Convention Center
Halls I, II, III

Specific Effect(s) in Chemical Reactions by Innovative Technologies (#157)

Organized by: S. Horikoshi, N. Serpone, R. Gupta, Y. Hayashi, M. Ashokkumar, M. Watanabe

Poster Session 19:00 – 21:00

600. Synthesis of large scorodite particles using ultrasound irradiation. **Y. Kitamura***, H. Okawa, K. Sugawara

601. Synthesis of calcium carbonate using CO_2 absorbed monoethanolamine and calcium chloride under ultrasonic irradiation. **T. Fujiwara***, H. Okawa, K. Sugawara

602. Hydrogen evolution from organic hydrides through microwave selective heating in heterogeneous catalytic flow systems. **M. Kamata**, S. Horikoshi*

603. Design of the catalyst most suitable for microwave organic hydride method. **Y. Kassai**, M. Kamata, S. Horikoshi*

604. Reply of microwave specific stress in the genetic level of the plant. **Y. Hasegawa**, N. Suzuki, S. Horikoshi

605. Change of chemical structure and activation of metalloenzyme by the microwave specific effect. **K. Nakamura**, M. Kawaguchi, J. Kondo, S. Horikoshi

606. Microwave effect in the intramolecular reaction using Claisen Rearrangement. **T. Watanabe**, Y. Suzuki, S. Horikoshi

607. Photolysis of VOC using microwave discharged electrodeless lamp (MDEL) technique. **K. Oshima**, A. Tsuchida, S. Horikoshi*

608. Fate of constituents of concern in water reclamation facilities in Korea. S. Park, Y. Son, **W. Lee***

609. Trial for electrodeless of the microwave induced plasma in liquid. **S. Sato***, K. Mori, O. Ariyada, H. Tsukamoto, T. Yonezawa

610. Direct conversion of methane and carbon dioxide by surface discharge non-equilibrium plasma reaction. **T. SUGAWARA***, H. ARITANI, A. OGATA

611. Synthesis of hydroxyapatite utilizing a interface reaction field between solid and liquid phases. **H. TAKAHARI***, Y. Wada, N. Yamamoto, M. Matsumoto, K. Onoe

612. Liquid phase purification by plasma-jet process utilizing activation of water droplets. **H. NISHIYAMA***, Y. Wada, N. Yamamoto, K. Onoe

613. Synthesis of porous iron oxide and its Adsorption characteristics. **T. OSAWA***, H. Okawa, K. Sugawara

614. New synthesis method of hydroxyapatite using a combined system of atmospheric pressure plasma with minute droplets. **K. Kudo**, Y. Wada, M. Matsumoto, K. Onoe

615. Development of generation technique of active oxygen species for efficient water purification. **R. Hatano**, Y. Wada, K. Onoe

616. Application of microbubble technique to antisolvent crystallization of glycine polymorphs. **M. Matsumoto***, Y. Wada, K. Onoe

617. Novel CO_2 -philic catechol derivatives for the $\text{Sc}-\text{CO}_2$ metal extraction. **h. kim**, **X. Yan**, **y. oh**

618. Solid-supported nanometal catalyzed hydrogenation in supercritical CO_2 . **h. kim**, **n. hur**, **j. yu**, **b. lee**, **k. lee**, **s. ahn**, **H. Song**

619. Bottom-up synthesis of mono-layer graphene by hydrothermal electrolysis. **Y. Okamura**, T. Tomai*, I. Honma

620. Selective recovery of magnesium from simulated concentrated sea water with continuous reactive crystallization in supercritical water using micromixer. **T. Sato**, A. Yano, M. Matsumoto, M. Okada, T. Hiaki*

621. Control of morphology and dispersibility of Boehmite nanoparticle modified by carboxylic acid in supercritical water. **T. Fujii***, S. Kawasaki

Hawaii Convention Center
Halls I, II, III

Natural to Nanosphere Lithographies: Two Decades of Self-assembled Advanced Materials (#177)

Organized by: A. Morfa, M. Giersig, K. Kempa, R. Duyne, L. Zhi

Presiding: E.M. Akinoglu

Poster Session 19:00 – 21:00

622. Study on the mechanism of particle nano-indentation and nano-imprinting in terms of the interaction between particles and substrates. **K. Yamamoto**, Y. Fukui, K. Fujimoto*

Hawaii Convention Center
Halls I, II, III

Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223)

Organized by: D. Jiang, W. Wang, W. Zhang

Presiding: D. Jiang, W. Wang, W. Zhang

Poster Session 19:00 – 21:00

623. Toward porous molecular crystals of single molecule magnets based on lanthanide phthalocyanine sandwich complexes. **L. Burt**, C.G. Bezzu, S. Mogach, N. McKeown

624. Covalent organic frameworks as chemosensors. **S. Ding**, M. Dong, Y. Wang, W. Wang

625. Covalent organic polymers (COPs) for energy conversion and storage. **Z. Xiang**

626. Preparation and use of orange and pineapple peels as adsorbents for pollutant removal from water. **L.V. Gonzalez-Gutierrez***, L.A. Romero-Cano, L.A. Baldenegro-Perez

627. Covalent organic frameworks with robust stabilities and tunable pore sizes. **S. Tao**, **H. Xu**, **D. Jiang**

628. New nanoporous aramid fiber aerogel. **K. Hirogaki***, D. Lei, I. Tabata, T. Hori

629. Separation of hydrogen isotopes by MOFs. **M. Hirscher***, I. Weinrauch, H. Oh, D. Denysenko, D. Volkmer, I. Savchenko, T. Heine

630. Porous-aromatic-frameworks (PAFs) for separation and storage applications. **K. Konstas***, C. Lau, A.J. Hill, M.R. Hill

631. Layer-by-layer growth of 3D covalent bonded networks via spontaneous urea coupling reaction. **S. Laakroekkiat**, M. RASHED, M. Hara, S. Nagano, Y. Nagao*

632. Application of electrode interlayers for highly efficient polymer solar cells. **F. Li**

633. Flexible macroporous polymer cages as spacer/spring elements for REWOD energy harvesting devices. **A. Menner**, Q. Jiang, A. Bismarck

634. One-pot Suzuki-Heck reaction to construct luminescent microporous organic polymers based on 4-vinylphenylboronic acid. **Z. Liang***, X. Song, J. Yu

635. Supramolecular imidazolium frameworks: Open analogs of metal azolate frameworks with node-and-linker polarity inversion. **C. Mottillo**, T. Friscic

636. 2D/3D COF nanostructures: From structural design to practical applications. **R. Mas-Balleste***, F. Zamora

637. Design and synthesis of triangular covalent organic frameworks. **P. Wang***, D. Jiang

638. Nano/meso-porous materials from block copolymer template using supercritical carbon dioxide: The relationship between porous structures and swelling in CO_2 . **T. Shinkai**, K. Ito, K. Sugiyama, H. Yokoyama*

639. Porous covalent organic materials made from polycyclic aromatic hydrocarbons. **R.A. Smaldone***

640. Facile low-cost strategy towards conjugated microporous hypercrosslinked polymer. **L. Tan***, B. Tan

641. Mechanized metal-organic frameworks. **L. Tan**, **Y. Yang***

642. Click-based porous organic frameworks for heterogeneous catalysis. **L. Li**, H. Zhong, **R. Wang***

643. Soluble, microporous, shape-persistent ladder polymers: Structure-property relationships and applications. **Y. Xia***

644. Covalent organic frameworks on carbon nanotubes for synergistic lithium-ion battery energy storage. **F. Xu**, D. Wu, R. Fu, D. Jiang*

645. Highly stable covalent organic framework for carbon dioxide capture with controlled loading functional groups via click chemistry. **L. Zhai**, **N. Huang**, **D. Jiang**

646. Photocatalytic water oxidation by carbon nitride polymers modified with cobalt cocatalysts. **g. zhang**, x. wang

647. High accuracy and high efficiency multi-scale simulations of the gas adsorption in porous molecular materials. **J. Zhang***

648. Ultralight, elastic, cost-effective, and highly recyclable superabsorbent from microfibrillated cellulose fiber for oil spillage cleanup. **S. Wang**, **L. Zhong**, X. Peng, R. Sun

649. Water sorption hysteresis modeling as a tool to elucidate wood cell-wall architecture. **S. Avramidis***, J. Shi*

650. In vitro hydrolytic degradation of biodegradable poly(L-lactic acid) blend monoliths. **Y. Nakamura***, H.T. Oyama, K. Uetani

Hawaii Convention Center
Halls I, II, III

Nanomaterials for Nanomedicine (#289)

Organized by: A. Maruyama, D. Lee, R. Narain

* Principle Author

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<http://pacificchem.org/onlineprogram>

Poster Session

19:00 – 21:00

- 651.** Development of enzyme-loaded polyion complex vesicles for *in vivo* nanoreactor. **Y. Anraku***, M. Kamiya, S. Tanaka, T. Nomoto, K. Toh, Y. Matsumoto, S. Fukushima, D. Sueyoshi, A. Kishimura, M.R. Kano, Y. Urano, N. Nishiyama, K. Kataoka
- 652.** Design of dual stimuli-responsive gel particles as nanotransporters for intracellular delivery. **A. Kawamura**, S. Ueno, T. Miyata*
- 653.** Direct evaluation of cell membrane integrity using ion-sensitive field-effect transistor. **Y. Imaizumi***, T. Goda, A. Matsumoto, Y. Miyahara
- 654.** Enhancement of blood circulation and tumor accumulation of a tumor imaging fluorescent probe by human serum albumin mediation. **e. nakhai***, C. Kim, D. Funamoto, T. Mori, A. Kishimura, Y. Katayama
- 655.** DNA structures stabilized with poly(ethylene sodium phosphate). **R. Moriyama***, D. Miyoshi, Y. Iwasaki
- 656.** Preparation of polymer nanosheets containing phosphorylcholine group and the application to coating biomaterials. **Y. Nagase***, Y. Okamura, K. Asao, A. Iwano
- 657.** Development of a novel enzymatic nano-reactors as biodetoxification nanomedicine. **H. Tang***, Y. Sakamura, S. Tanaka, T. Mori, Y. Katayama, A. Kishimura
- 658.** Chelator-free radiolabeling of gold nanoclusters for accurate cancer diagnosis. Y. Zhao, L. Detering, D. Sultan, H. Luehmann, **Y. Liu***
- 659.** Reversible coating of liposome with serum albumin for improved blood circulation. **H. Sato**, Y. Nakamura, Y. Tahara, Y. Tatsuhiro, A. Kishimura, T. Mori, Y. Katayama
- 660.** Silica and polymer nanocapsules: A route to the stimulus responsive delivery of small molecules, polymers, and gases. **J. Kumar***, C. Liu, Y. Liu
- 661.** Fascinating composites based on bacterial cellulose for nanomedicine. **G. Yang***, Z. Shi, Y. Li
- 662.** Magnetic-plasmonic hybrid Ag@FeCo@Ag core@shell@Shell nanoprobes for isolation of intracellular membrane vesicles. **M. Takahashi**, P. Mohan, K. Higashimine, A. Nakade, D.M. Mott, T. Hamada, K. Matsumura, T. Taguchi, S. Maenosono*
- 663.** Surface-initiated atom transfer radical polymerization from various materials reacted with a photoreactive initiator. **K. Fukazawa***, K. Ishihara
- 664.** Development of photothermal cancer therapy using gold nanorods. **T. Oikawa***, K. Gonda, Y. Kubota, Y. Kobayashi, M. Takano, T. Kamei, N. Ohuchi
- 665.** Application of novel hetero-tagged angiogenic factors to *in vivo* fluorescent imaging with high resolution. **Y. Hamada***, T. Okawa, K. Gonda, N. Ohuchi
- 666.** Photofunctional nanomodulators for bioexcitation. **E. Miyako**
- 667.** Design of biocompatible polymeric gene carrier utilizing serum albumin. **Y. Nakamura***, H. Sato, T. Yoshikawa, Y. Tatsuhiro, A. Kishimura, T. Mori, Y. Katayama
- 668.** Protein adsorption at well-characterized polymer brush surfaces based on molecular interactions. **Y. Inoue***, S. Sakata, K. Ishihara
- 669.** Design and functions of new immunoliposomes by *in vitro* protein synthesis/artificial cell system. **M. Ando***, R. Miura, S. Mukai, Y. Akahori, S. Sawada, H. Shiku, Y. Sasaki, K. Akiyoshi
- 670.** Nanoplasmionic microplate based on Au@Ag NPs for multiplex pathogen detection. **H. Gil**, S. Kim, J. Ryu, S. LEE*
- 671.** Immunomodulatory liposomal spherical nucleic acids. **N. Chernyak**, M. Guan, A.J. Sprangers, S. Narajan, C.A. Mirkin*
- 672.** AuNs@Au nanoparticle as SERS nanoprobe for multiplex cancer diagnosis. **J. Ryu**, N. LEE, H. Gil, S. LEE*

- 673.** Novel nanoparticle-mediated combinatorial therapy against triple negative breast cancers. **D. Ho***, A. Sorolla*, C. Ormonde, E. Wang, C.W. Evans, K. Iyer, P. Blancafort
- 674.** Creation of nano-prodrugs and their cytotoxic activities. **H. KASAI***, Y. Koseki, Y. Ikuta, T. Onodera, H. Okawa
- 675.** Intravenous delivery of albumin-conjugated nanoparticles to the brain following a remote injury in the central nervous system. **n. smith***, I. Gachulinova, D. Ho, C. Bailey, C. Bartlett, M. House, M. Fitzgerald, K. Iyer, S.A. Dunlop
- 676.** Amplifying the effective binding affinity of carbon nanotube biosensors to cancer cells by control over antibody orientation and density. **H. Kim**, D. Hwang, S. Jeon, J. Chung, J. Kim*
- 677.** Upper critical solution temperature (UCST) type thermo-responsive micelles covered with biocompatible shells. **A. Fujihara***, S. Yusa, A. Maruyama, N. Shimada, K. Ishihara
- 678.** Enhanced Immunostimulation for cancer vaccine with crosslinked CpG-ODN/β-1,3-glucan nanogel through hybridization. **N. Miyamoto***, K. Sakurai, S. Mochizuki
- 679.** Preparation of macrophage-specific magnetite nanoparticles by modifying with gelatin. **T. Niidome***, E. Makiyama, J. Matsuyama, T. Kida, Y. Komohara, M. Takeya
- 680.** Enhanced catalytic activity of chemically modified 10-23 DNase by cationic comb-type copolymers. **K. Saito**, N. Shimada, A. Maruyama*
- 681.** Studies on functionalization of Hemagglutinating Virus of Japan Envelope (HVJ-E) with layer-by-layer assembly technique. **T. Okada***, K. Uto, C. Lee, T. Aoyagi, M. Ebara
- 682.** Synthesis of biocompatible polyimide containing PC group and fabrication of nanosheet as a coating agent. **M. Ogino**, K. Asao, Y. Okamura, Y. Nagase*
- 683.** Design of stimulus-sensitive polyrotaxanes exhibiting their supramolecular dissociation in response to metabolic acidosis. **K. Nishida**, A. Tamura, N. Yui*
- 684.** Fabrication of biodegradable spherical particles and fibers by SPG membrane emulsification technique. **A. Nakagawa**, Y. Okamura
- 685.** Intracellular protein delivery using ganglioside GM1-binding peptide. **H. Maeno***, T. Matsubara, T. Sato
- 686.** Hemoglobin-loaded photoresistor nanoparticles for improved photodynamic therapy. **C. Li**, H. Hao, P. Lai
- 687.** Preparation and characterization of UCST-type thermo-responsive polypeptide as smart biomaterials. **S. kuroyanagi**, N. Shimada, A. Maruyama*
- 688.** Smooth muscle differentiation related transcription factor CRP2 directly regulates structure and dynamics of actin filaments. **T. Kihara***, S. Takaoka, S. Shinohara, J. Miyake
- 689.** Multifunctional mesoporous silica nanoparticles for photothermally-triggered doxorubicin release to overcome drug-resistant MCF-7/ADR cells. **J. Jian**, C. Chen , P. Lai
- 690.** Synthesis of biocompatible polyurethane and fabrication of nanosheet as a coating agent. **A. Iwano**, K. Morita, K. Asao, Y. Okamura, Y. Nagase*
- 691.** Evaluation of PEG-modified β-glucans for efficient delivery to specifically cancer. **D. Ito**, S. Mochizuki, y. maegawa, K. Sakurai*
- 692.** Enhanced photodynamic efficacy by gas/PFD encapsulated nanoparticles. **R. Chen**, C. Liu, P. Lai
- 693.** Development of vascularized iPSC derived 3D-cardiac myoblast tissues by filtration layer-by-layer technique. **Y. Amano**, A. Nishiguchi, M. Matsusaki, M. Akashi*
- 694.** Synthesis of influenza virus-recognizing glycopolymer via RAFT polymerization and copper-catalyzed azide-alkyne cycloaddition. **M. Nagao**, H. Seto, T. Tanaka, Y. Hoshino, Y. Miura*
- 695.** Water-soluble complex with biocompatible polymer and fullerene as photosensitizer. **T. Ohata**, S. Yusa, K. Ishihara
- 696.** Preparation of polysaccharide modified micelles for cell specific gene delivery. **M. Ishida**, S. Mochizuki, I. Fukuda, K. Sakurai*
- 697.** Macrophage targeting gene delivery using micelle composed of mannose and cationic lipids. **I. Fukuda***, S. Mochizuki, K. Sakurai
- 698.** Development of biodegradable multi-layered nanosheets as a wound dressing in partial hepatectomy. **T. Komachi**, H. Sumiyoshi, Y. Inagaki, S. Takeoka, Y. Nagase, Y. Okamura*
- 699.** Selenium-platinum complexes selectively kill cancer cells via ROS. **T. Li**, H. Xu*
- 700.** Efficient delivery of nucleic acid medicines using pH responsive pyramidal DNA. **S. Tokunaga***, S. Mochizuki, N. Miyamoto, K. Sakurai
- 701.** Hyaluronic acid-grafted polyamidoamine dendrimers enable active tumor targeting and long circulation in vivo. **X. Qi**
- 702.** Biodegradation of carbon nanohorns. **M. Zhang***, M. Yang, C. Bussy, S. Iijima, K. Kostarelos, M. Yudasaka
- 703.** Activation of the membrane-disrupting peptide by the cationic polymer. **W. Sakamoto**, T. Umegae, N. Kume, N. Shimada, A. Maruyama*
- 704.** Synthesis and biocompatibility of polyurethane containing phosphorylcholine and alkyl groups. **M. Tezuka**, A. Iwano, K. Morita, Y. Okamura, Y. Nagase*
- 705.** Physicochemical characterization of hyaluronan nanoparticles and their interaction with cells. **N. Tsuji***, T. Sato
- 706.** Adsorption mechanism and structure of DNA on graphene oxide nanosurface. **Y. Ueda**, Y. Zouzumi, N. Sugimoto, D. Miyoshi*
- 707.** Molecular mechanism of metallofullerenol $Gd@C_{62}(OH)_{22}$ in anti-metastasis of pancreatic cancer: *In silico* modeling of of nanomedicine. **S. Kang***, T. Huynh, R. Zhou
- 708.** pH-Responsive nanoclusters for magnetic resonance imaging, photothermal therapy and overcomes multiple drug resistance. **C. Lin**, Y. Cheng, M. Huang, P. Lai
- 709.** Preparation of Co-ferrite nanoparticles and effect of hyperthermia treatment. **I. Ohta**, Y. Ichiyanagi
- 710.** Preparation of functional magnetic nanoparticles and mass spectroscopy imaging. **S. Morimoto***, K. Hyodo, T. Yamazaki, T. Ishikawa, Y. Ichiyanagi
- 711.** Antibody-conjugated pluronic nanogel for active targeting diagnosis and therapy of cancer. W. Choi, j. lee, J. Kim, S. Heo, Y. Jeong, Y. Kim, **G. Tae***
- 712.** Bundle assembly of double stranded DNA using β-cyclodextrin-modified naphthalene diimide and bisadamantyl piperazine. **R. Moriyama**, S. Sato, S. Takenaka
- 713.** Development of multifunctional dendrimer-gold nanorod hybrids for photothermal chemotherapy. **T. Hashimoto**, E. Yuba, A. Harada, K. Kono*
- 714.** Quantitative evaluation of intracellular trafficking using pDNA/chitosan/nanoparticles. **A. Shimatani**, T. Sato*
- 715.** Novel mouse xenograft model for *in vivo* imaging in a nanomedicine field. **S. Kita**, H. Higuchi
- 716.** Enhancement of the adjuvant activity of dsRNAs by conjugation with gold nanoparticles. **T. Tazaki***, K. Niikura, T. Suzuki, Y. Ohara, S. Kobayashi, T. Nakano, Y. Orba, H. Mitomo, H. Sawa, K. Ijiro
- 717.** Cell uptake of liposomes modified with GM3-binding peptide. **M. Fujimoto**, T. Kimura, J. Kim, R. Otani, T. Matsubara, T. Sato
- 718.** Preparation and characterization of thermo-responsive polymer modified liposomes aimed at application to anticancer agent delivery. **R. Nemoto***, J. Wang, Y. Hiruta, A. Eri, Y. Maitani, H. Kanazawa
- 719.** Characterization about thermosensitive liposome and make an effective cellular uptake. **J. Wang***, R. Nemoto, A. Eri, Y. Hiruta, Y. Maitani, H. Kanazawa
- 720.** Hydration structure at molecular hydrophobic interfaces in O/W type surfactant free nano-emulsion. **Y. Yawaza***, M. Kato*, T. Eguchi
- 721.** Physical properties of SPG/ODN complex revealed by gel permeation chromatography and small angle X-ray scattering analyses. **S. Mochidome***, S. Mochizuki, K. Sakurai
- 722.** Solubilization at fullerene in water by thermo-responsive diblock copolymer. **J. Yano***, S. Yusa, T. Ohata, K. Ishihara
- 723.** Spray-nano-coating of fragmented biodegradable nanosheets for biomedical applications. **S. Takano**, H. Sumiyoshi, Y. Inagaki, H. Kimura, Y. Okamura*
- 724.** Fabrication of disk-shaped particles induced by hot-press process and their 2D interactions for biomedical applications. **D. Sogabe**, Y. Nagase, Y. Okamura
- 725.** Platinum based chemotherapeutic agents and holmium containing magnetic nanoparticles for targeted treatment of non-small cell lung cancer. i. munaweera, Y. Shi, B. Koneru, r. saez, A. Ali , A. Di Pasqua, **K. Balkus***
- 726.** Targeted nanoparticles for improved vaccine delivery. **A.P. Johnston***, J.D. Mintern
- 727.** Fat-targeted delivery of thiazolidinediones as antidiabetic drugs. **K. SAATCHI**, E. Dunn, S. Tod, K. Nicholson, D. Leung, I. Andreu, C. Buchwalder, V. Schmitt, U. Hafeli, S. Gray*

Hawaii Convention Center
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Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308)

Organized by: R. Morandotti, D. Moss, F. Omenetto, N. Tsutsumi, K. Alamgir, K. Char, A. Facchetti

Poster Session

19:00 – 21:00

- 728.** Large-area, cost-effective plasmonic nanostructures based on nanotemplates. **D. Choi***, J. Kwon, K. Chung
- 729.** Two-photon polymerization of negative-type photoresist. **T. Miura**, K. Kinashi, W. Sakai, N. Tsutsumi
- 730.** Novel acid amplifiers for UV or EUV lithography with high photosensitivity and resolution. **K. TAKAHASHI**, M. Furutani, K. Arimitsu*
- 731.** Degradation studies of methylammonium lead iodide perovskite solar cells. **E.M. Sanehira***, B.J. Tremolet de Villiers, L.Y. Lin, J.J. Berry, J.M. Luther
- 732.** Electroluminescence of $CaTiO_3/Bi/In_2O_3$ multilayer thin films prepared by a sol-gel method. **Y. Hayashi***, T. Kyomen, M. Hanaya, H. Takashima
- 733.** Holographic property of carbazole azobenzene composite films. **Y. Yabuhara***, K. Kinashi, W. Sakai, N. Tsutsumi
- 734.** Synthesis and property of calixarene-containing polymers and their application for photo-resist material. **O. Hiroki***

* Principle Author

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- 735.** Synthesis and characterization of fullerene derivatives with carboxylic acid ester in organic photovoltaic devices.
M. Igawa, K. Abe, H. Lee, J. Lee, J. Jang, C. Pac, H. Moriyama*
- 736.** Holographic property in PMMA composites doped with carbazole azobenzene compound with different electron accepting substituent. **S. Motoishi***, K. Kinashi, W. Sakai, N. Tsutsumi
- 737.** Organic thin film dye laser device with DBR structure. **S. Nagi**, K. Kinashi, W. Sakai, N. Tsutsumi
- 738.** Detecting methylation in arginine using optical microresonators. **A. Rios**, V. Sun, C. Zurita-Lopez, A. Armani
- 739.** Combined total scattering and density functional theory studies of amorphous indium gallium zinc oxide. **D. Fast**, B. Hanken, P.H. Cheong, M. Dolgos
- 740.** Theoretical investigation on the charge transport in high-mobility organic semiconductors. **J. Yuqian**
- 741.** Dry process photopatterning of a conducting polymer using photoinduced acid proliferation reactions. **S. Kubodera**, M. Furutani, K. Arimitsu*
- 742.** Photoreduction of metal ions through two-photon excitation in polymer matrix. **R. Nakamura***, K. Kinashi, W. Sakai, N. Tsutsumi
- 743.** Development of high-response photorefractive device with main-chain triphenylamine polymer. **K. Kono***, S. Tsujimura, K. Kinashi, N. Tsutsumi
- 744.** Synthesis and properties of halogenated subnaphthalocyanines for organic photovoltaic cells. **Y. Takao***, T. Matsuka, K. Yamamoto, T. Mizutani, J. Matsumoto, K. Moriwaki, T. Iwai, T. Ito, T. Mizuno, T. Ohno
- 745.** Effect of crystallization of nonlinear optical dye in organic photorefractive composites: Enhanced photoconductivity and change of the density of states. **S. Tsujimura**, T. Fujihara, T. Sassa, K. Kinashi, W. Sakai, K. Ishibashi, N. Tsutsumi*
- 746.** Ferroelectricity of thin film of vinylidene fluoride-trifluoroethylene copolymer doped with nanoparticles. **R. Kosugi***, K. Kinashi, W. Sakai, N. Tsutsumi
- 747.** Video rate response photorefractive devices by changing the plasticizer concentration. **T.V. NGUYEN***, H.N. GIANG, K. Kinashi, W. Sakai, N. Tsutsumi
- 748.** Plasmonic metallic films covered with graphene layers. **J. Park***, H. Hong, K. Shin, S. Lee
- 749.** Development of organic solar cells based on low-bandgap π -conjugated molecules. **Y. Hidaka**, W. Shin, T. Yasuda*
- 750.** Fabrication of centimeter-sized thin-layered colloidal crystals. **K. Ito***
- 751.** Hybrid perovskite solar cells using functional ligand (II): Optical properties of perovskites containing fullerene derivatives. **M. Imada**
- 752.** Synthesis and characterization of self-doped conjugated diblock copolymers (I): Effect of side chain of thiophene. **T. Hazeki**, M. Fujita, Y. Takeoka, M. Rikukawa
- 753.** Patterned taping: A novel and high-efficiency soft lithographic method for organic thin films. **S. Oh**, S. Park, J. Kim, I. Cho, S. Park*
- 754.** Terminal functionalized diketopyrrolopyrrole-based small molecules for organic photovoltaic devices. **S. Furukawa**, H. Komiyama, T. Yasuda*
- 755.** Preparation of highly conductive and flexible graphene hybrid fibers for wearable electronic applications. **J. Lee***
- 756.** Study of bending-resistance for flexible organic solar cell. **D. Kato**, A. Aoki, T. Abe
- 757.** Series of non-fullerene dye-based small molecule acceptors in OPVs showing PCEs over 3%. **E. LIM**
- 758.** Development of efficient blue thermally activated delayed fluorescence emitters and clarification of concentration quenching mechanism. **J. Lee**, M. Numata, W. Shin, Y. Yang, C. Adachi, T. Yasuda*
- 759.** Ultra-conformable polymer nanosheets with inkjet-printed electric circuits. **M. Okamoto**, T. Fujie, M. Kurotobi, K. Yamagishi, A. Murata, E. Iwase, H. Iwata, S. Takeoka
- 760.** Boosting the efficiencies of cost-effective perovskite solar cells by interfacial engineering with rod-like CuPc. **X. Yang***, X. Yang*, M. Cheng, W. Wang, L. Sun*
- 761.** Fabrication of transparent organic thin film solar cell. **Y. Matsumoto**, A. Aoki, T. Abe
- 762.** Novel and facile fabrication of organic solar cells by incorporating self-organized hole transport layer. **D. Kim**, O. Kwon, S. Park
- 763.** Transient photocurrent of organic photovoltaics assisted by electric double layers in electrolytes. **M. Odaka***, M.M. Matsushita, K. Awaga
- 764.** Emitting materials for thermally activated delayed fluorescent organic light-emitting diodes using benzothiophazole and acridine moieties. **J. Jun**, C. Lee, O. Kim, S. Hwang*
- 765.** Small bandgap polymer solar cells with unprecedented short-circuit current density maintaining high fill factor. **H. Choi***, S. Ko, P. Morin, M. Leclerc, J. Kim, A.J. Heeger
- 766.** Controllable metal-to-insulator transition in electroless-deposited Au nanofeatures on silicon substrate. **J. Jang**, S. Lee, S. Hwang
- 767.** Preparation and photoconductive properties of Ag nanoparticles grown in TiO_2 nanropes. **K. YAMAZAKI**, T. ISHIDA, T. MUSHA, M. Fujino*, H. KATAGIRI, G. KAWAMURA, A. MATSUDA
- 768.** Asymmetrical squaraines bearing fluorine-substituted indoline moieties for high-performance solution-processed small molecular organic solar cells. **D. Yang**, Y. Huang*, Z. Lu, H. Sasabe
- 769.** Control of photothermal effect in metallic nanoparticle-assembled system for detecting biochemical substances. **Y. Nishimura**, Y. Yamamoto, S. Ito, S. Tokonami, T. Iida*
- 770.** Negative resistance of Ag nanoparticles dispersed in quinacridone matrices. **Y. Masuda**, Y. Ishizeki, H. Ivy, M. Fujino*
- 771.** Soft X-ray spectroscopy on insulating rutile phase of niobium doped VO_2 thin films at low temperatures and ambient pressures. **T. Su***, J. Laverock, V. Jovic, K.E. Smith, S. Kittiwatanakul, J. Lu
- 772.** Clarification of Si added a-C characters that contribute high efficiency solar cell and improvement of its semiconductor properties. **Y. Nagata***, M. YAMADA, R. Kobayashi, K. Honda
- 773.** Solution-processed oxide thin film phototransistor by polymer pre-pattern. **J. Choi**, K. Kim, s. park, D. You, Y. Kim*
- 774.** Effects of resonant bonding in $Sn_2Sb_2Se_5$ phase change materials. **M. Ahn**, K. Jeong, S. Park, S. Park, J. Han, W. Yang, M. Jang, H. Jeong, M. Cho*
- 775.** Antiaromatic nororrole batteries. **J. Shin***, T. Yamada, H. Yoshikawa, K. Awaga, H. Shinokubo
- 776.** Solution processed hafnia thin-film as a capping layer for enhanced dehydration of thin-film dielectrics. **C.K. Perkins**, R.H. Mansergh, D. PARK, Y. Huang, S.R. Decker, D.A. Keszler
- 777.** Mechanofluorochromic behaviors of 1-alkanoylaminopyrenes. **E. Nagata***, S. Takeuchi, T. Nakanishi, Y. Hasegawa, Y. Mawatari, H. Nakano
- 778.** Reversible color change of hybrid films composed of azobenzene-based amorphous molecular materials and p-toluene sulfonic acid. **R. Ichikawa**, E. Nagata, H. Nakano*
- 779.** Response change at interdigitated array microelectrodes consist of boron-doped amorphous carbon by varying geometry for high sensitive detection of redox analytes. **K. Honda***, S. Ohtomo, Y. Nagata, M. YAMADA, R. Kobayashi
- Hawaii Convention Center
Halls I, II, III**
- Data Mining and Machine Learning Meets Experiment and First-Principles Simulation for Materials Discovery (#314)**
- Organized by:** J. Schrier, C. Amador-Bedolla, S. Iwata, T. Woo
Presiding: C. Amador-Bedolla, S. Iwata, J. Schrier, T. Woo
- Poster Session
19:00 – 21:00**
- 780.** In-silico prediction and screening of ABC-6 zeolites: A high-throughput genomic approach. **Y. Li***, J. Yu*
- 781.** Simulation-based data-mining approach for the protein hydration water behavior. **T. Mizukami**, V. Nguyen, T. Ho, H. Dam
- 782.** Prediction of interface structure and energy with an aid of information science. **S. Kiyohara***, T. Mizoguchi
- 783.** Linear representation for calculating atomic forces. **T. Pham***, H. Dam*
- 784.** Sparse modeling for materials design. **H. Dam***, T. Pham*, V. Nguyen
- Hawaii Convention Center
Halls I, II, III**
- The Physical Structure, Function of Biological and Bioinspired Soft Matter (#347)**
- Organized by:** M. Srinivasarao, A. rey, H. Jung
- Poster Session
19:00 – 21:00**
- 785.** Stochastic delay-derivative device elements using binary mixtures containing biobased polymers: Potential application for bioinspired signal processing devices with hierarchical instabilities. **R. Maruyama**, N. Asakawa*
- 786.** Surface observations and friction measurements of *Thermobia domestica*'s scales. **N. Okuda***, Y. Hirai, M. Shimomura
- 787.** Role of cross links on collagen fibril orientation in pericardium. **H.R. Kayed***, N. Kirby, A. Hawley, S. Mudie, R.G. Haverkamp
- 788.** Preparation of artificial plastrons by using self-organized honeycomb-patterned film. **N. Yanagi**, Y. Hirai*, M. Shimomura
- 789.** Fabrication of the durable shark skin mimicking surface by using self-organized structures. **A. Sato***, Y. Hirai, T. Ohzono, K. Suzuki, S. Koike, T. KUROKAWA, M. Shimomura
- 790.** Structure of water and polymer network in poly(vinyl alcohol) hydrogels with repeated freezing-thawing cycles. **Y. Sekine**, N. Ishikawa, T. Ikeda-Fukazawa
- 791.** Preparation of hybrid materials from spider silk and conducting polymers. **K. Miyaura**, O. Karthaus*
- Hawaii Convention Center
Halls I, II, III**
- Safety and Sustainability of Nanotechnology (#404)**
- Organized by:** Y. Zuo, J. Ferri, C. Chen, J. Loo, S. Mylon
- Poster Session
19:00 – 21:00**
- 792.** Lung surfactant as a target for zinc oxide nanoparticle toxicity. **E. Da Silva***, S. Larsen, J.B. Sorli
- 793.** Probe the interactions between inhaled nanoparticles and model pulmonary surfactant: Insights from molecular dynamics simulation. **X. Lin***, Y. Zuo, N. Gu
- 794.** Response of rat alveolar macrophages upon in vivo exposure to silver nanowires. **E. Ogorodnik***, G. Liu, Y. Liu, A. Karsali, L.M. Franz, A.K. Pham, I. Espiritu, K.E. Pinkerton
- 795.** Near-infrared light-mediated nanomaterials as a precision nanomedicine. **C. Chen**
- Hawaii Convention Center
316C**
- In vitro simulation of carbon nanotube and graphene impact on lung surfactant. Y. Zuo***
- Hawaii Convention Center
316C**
- Single-Molecule Function and Measurements (#408)**
- Organized by:** T. Ogawa, H. Tada, S. Park, P. Weiss
Presiding: T. Matsumoto
- 19:00 – 797.** Chirality effects of SWNTs on the supramolecular structures of porphyrin derivatives on the curved surfaces. **A.I. Abd El-Mageed**, G. Liu, N. Komatsu, T. Inose, T. Ogawa*
- 19:20 – 798.** Structural defects control of multiwall carbon nanotubes using statistical strategies for electrochemical detection of glucose. **A. TermehYousefi**, H. Tanaka
- 19:40 – 799.** Photoelectronic functional DNA nanowires stretched between electrodes toward DNA molecular device. **N. Kobayashi***, T. Kunikyo, N. Nakamura
- 20:00 – 800.** Direct observation of single-molecule adsorption/desorption kinetics on ion-exchange adsorbents. **S. Dharmane, L. Kisley, M. Poongavanam, U. Patil, A. Mansur, S. Dominguez-Medina, E. Kulla, W. Chen, J. Chen, K. Kourentzi, C.F. Landes*, R.C. Willson***
- 20:20 – 801.** Design, synthesis, and characterization of ambipolar organic molecules with cascaded energy level for long-lived charge separated states. **T. Wang***, D. Liu, X. Zhou, W. Li, K. Weerasingham, L. Wang
- Hawaii Convention Center
317B**
- The Frontiers of Geometrically Frustrated Magnetic Materials (#430)**
- Organized by:** C. Wiebe, C. Ling, J. Gardner, H. Zhou
- 19:00 Introductory Remarks**
- 19:05 – 802.** Crystal chemistry and magnetic interactions in frustrated copper minerals. **Z. Hirai***, K. Nawa, H. Ishikawa
- 19:45 – 803.** Complex field induced phases in the frustrated quantum spin chain ilünlite. **K.C. Rule***, B. Willenberg, S. Nishimoto, M. Schäpers, M. Reehuis, A. Wolter-Giraud, S. Drechsler, B. Buchner, A. Studer, B. Ouladdiaf, S. Stollw
- 20:25 – 804.** Short-range magnetic interactions and optical band-edge physics in $SiCu_2(BO_3)_2$. J. Cherian*, T. Tokumoto, h. zhou, S. McGill
- 20:40 – 805.** Magnetic frustration in 2D lattices of bow-ties. **R. SIBILLE***, V. Simonet, E. LHOTEL, T. MAZET, B. MALAMAN, M. FRANCOIS
- Hawaii Convention Center
319B**
- Self-assembled Biofunctional Nanomaterials (#433)**
- Organized by:** R. Nagarajan, K. Sakurai, H. Chen
-
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- 19:00 – 806.** Systematic manipulation of DNA functionality by controlled self-assembly and disassembly. **T. Pfohl**
- 19:30 – 807.** Development of hetero-selective pseudo base pair stabilized by charge-transfer interaction, and its hetero-duplex formation. **T. Doi**, T. Sakakibara, H. Kashida, H. Asanuma
- 19:50 – 808.** Effect of various metal ions on self assembly of tyrosine-rich peptide and its applications as biosensors. **N. Lee**, S. Kim, H. Gil, S. Lee*
- 20:10 – 809.** Fabrication of 3D nanodot array using Dps-DNA self-assembly. **H. Kamitake***, M. Uenuma, N. Okamoto, Y. Ishikawa, I. Yamashita, Y. Uraoka
- 20:30 – 810.** Programmable anisotropic self-assembly of gold nanorods regulated by DNA terminal base pairing. **G. Wang**, Y. Akiyama, S. Shiraishi, T. Takarada, M. Maeda*

Thursday Morning

Hawaii Convention Center
Halls I, II, III

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi

Poster Session

10:00 – 12:00

- 811.** Colormetric detection of SQUAMOSA promoter binding protein-like 12 via DNA-modified AuNPs cluster. **J. Ahn**, J. Jung*, A. Lee, J. Lee
- 812.** Fabrication of the hollow polystyrene particles by ultraviolet irradiation. **S. Hayakawa**, T. Kawai
- 813.** Heteronuclear organometallic clusters as single-source precursors for the formation of bimetallic nanoparticles: Synthesis, structural characterization, and catalytic application. **B. Chor**, C. Choong, W.O. Moersole, R. Raja, L. Chen, W. LEONG
- 814.** Preparation and electrochemical performance of $Zn_3V_2O_7(OH)_2(H_2O)_2$ micro-flower as anode materials for lithium-ion battery. **Y. Jiang***
- 815.** Polydopamine attachment chemistry for fabricating functionalized nanoparticles. **K. Kartub***
- 816.** Synthesis, characterization, and modification of FeNd₃O₆ nanoparticles. **A. Reiber***
- 817.** Combination of thio-click, ROP, and ATRP methods to prepare nano-I-lactide-b-n,n-dimethylhydroxyethylacrylamide poss copolymers. **A.M. Haddad**, B. Al-Mayahi, H. Al-Lami
- 818.** Synthesis and magnetic properties of europium chalcogenide nanoparticles. **N. Rosa**, W.L. Boncher, M.A. McNamara, S.L. Stolt
- 819.** Fabrication of hybrid microspherical polymer particle with non-close-packed arrays of colloidal silica on surface. **N. Hano**, N. Ryu, M.A. Alam, S. Nagaoka, M. Takaishi*, H. Ihara*
- 820.** Controlled growth of poly(aniline-co-substituted aniline) nano/microstructures in-situ in the Michael addition reaction system. **J. Li***
- 821.** Development of novel radiosensitizing cancer therapy: Combination of radiotherapy and titanium peroxide nanoparticle. **K. Morita**, T. Suzuki, M. Nakayama, R. Sasaki, K. Sato, C. NUMAKO, C. Ogino, A. Kondo
- 822.** Carbon-coated V₂O₅ nanocrystals synthesized from metal organic framework (MIL-47) as a high performance cathode material for Li-ion batteries. **J. Kim***
- 823.** Preparation and characterization of nonosize polymer sphere. **D. Kim**, M. Song
- 824.** Preparation and characterization of Keratin/poly (vinyl alcohol) blended nanofibers by electrospinning. **T. Kim**, M. Park, H. Kim*
- 825.** Preparation and characterization of graphene via electron beam irradiation. **T. Kim**, M. Park, H. Kim*

- 826.** Preparation and characterization of aminophenol grafted and Ag NPs decorated graphene nanocomposites. **S. Chae**, M. Park, H. Kim*
- 827.** Facile preparation and characterization of human hair-based nanofibers via electrospinning. **S. Chae**, M. Park, H. Kim*
- 828.** Developing tailorredgold nanarchecture for imaging application. **Y. Wang**, A. Kakkar, F. Lesage
- 829.** Analysis of surface enrichment of graft copolymer with poly(trimethylene carbonate) and poly(ethylene glycol) oligo segment. **K. Nitta**, K. Atsushi, J. Watanabe, Y. Ikeda
- 830.** Control of nanoparticle dispersion using semi-flexible chains grafted to silica: Role of chain stiffness and grafting density. **K. Bornani**, B. Barkatky, B. Lokitz, J. Mays, S. Kilbey
- 831.** Ultrashort channel floating gate memory with a nanoparticle array utilizing biomaterial. **T. Ban**, M. Uenuma, S. Migita, N. Okamoto, Y. Ishikawa, I. Yamashita, Y. Uraoka
- 832.** Partial surface modification of spherical inorganic oxide particles using a silane coupling agent. **M. Ono**, R. Ai, T. Endo, K. Torigoe, K. Sakai, M. Abe, H. Sakai
- 833.** Amphiphilic glucan nanoball for drug delivery. **S. Takeda**, S. Sawada, Y. Sasaki, K. Akiyoshi
- 834.** Fluorescence dynamics of charge -transfer complex nanoparticles composed of N-ethylcarbazole with tetracyanobenzene. **S. Yasuda**, S. MACHIDA, N. Ikeda
- 835.** Grain size dependence of magnetic properties in L_{10} -FePd/ α -Fe nanocomposite magnets. **K. Matsumoto**, R. Sato, T. Trinh, N. Sakuma, T. Teranishi
- 836.** Hybrids formation from titania nanoparticles and polymers by surface-initiated ATRP with a new organophosphorus surface modifying agent. **K. Mori**, J. MOTOGANI, M. MINODA
- 837.** Synthesis of CdSe compound semiconductor nanoparticles using biological templates, apoferritin: The effect of artificial nucleation site. **K. Iwahori***
- 838.** Robust thermal decomposition synthetic route to noble bimetallic alloy nanoparticles. **E. Choi**, S. Lee, Y. Piao*
- 839.** Structural control of porphyrin face-coordinated gold clusters for constructing desired assemblies. **D. Eguchi**, M. Sakamoto, T. Teranishi
- 840.** Synthesis of core-shell particles containing peroxydes utilizing oxygen supply from a gas-liquid interface and their application to dismantlable adhesives. **E. Sato**, M. Yuki, S. Fujii, T. Nishiyama, Y. Nakamura, H. Horibe
- 841.** Phase transfer of Au nanoparticles using long chain amide derivatives. **Y. Sou**, M. Nakagawa, Y. IMURA, T. Kawai
- 842.** Development of self-assembled nano-hybrid of magnetic nanoparticles cluster accommodated in polysaccharide nanogels. **R. Kawasaki**, Y. Sasaki, K. Katagiri, S. Sawada, K. Akiyoshi
- 843.** Enzyme-magnetic nanoparticle conjugates as rigid biocatalyst for the elimination of toxic aromatic hydrocarbon. **J. Chang***
- 844.** Simple synthesis that is applicable to various metal(oxide) of asymmetric nanoparticles with controllable shape and property. **J. Koo**, I. Lee
- 845.** N-type flexible thermoelectric material: Double-layer structure from Bi₂Se₃ nanoparticles and poly(vinyl alcohol) matrix. **A. Ohnuma**, K. Iwasaki
- 846.** Formation of alkyl polyglycoside vesicles using boric acid-diol complexation. **Y. Asano**, T. Aikawa, T. Kondo, M. Yuasa*
- 847.** Mesoporous silica nanoparticles: Promising theranostic nanocarriers to overcome current limitations in the treatment of cancer and neurodegenerative disease. **M. Bouchouicha**, E. Beliveau, R. C.-Gaudreault, F. Calon, M. Fortin, F. Kleitz
- 848.** Oxygen reduction reaction by iron oxide nanorods coated with N-doped carbon as catalyst. **L. Hadidi**, E. Davari, T.K. Purkait, D. Ivey, J. Veinot
- 849.** Preparation of AuNPs dispersed in various organic solvents using a long-chain amidoamine derivative. **K. Fukuda**, T. Kawai
- 850.** Specific drug delivery for target cancer tumor using affibody-displaying bionano-capsule/liposome complex. **Y. Nishimura**, J. Ishii, C. Ogino, A. Kondo
- 851.** Performance enhancement of organic solar cells with gold nanoparticle clusters. **H. Park**, S. Lee, S. Han, S. Kim
- 852.** Urea biosensor based on NiO decorated cellulose nanocomposite. **N. Nhisa**, T. Tran, G. Das, H. Yoon*
- 853.** Preparation and catalytic oxidation properties of Au nanoparticles catalysts immobilized on thiol functionalized mesoporous materials. **T. Hakeda**, J. Nakazawa, S. Hikichi*
- 854.** Structural and physical properties of the Ni(dmit)₂ salts with size valuable dications. **A. Kimura**, H. Kubota, Y. Takahashi, J. Harada, H. Hasegawa, T. Inabe
- 855.** Preparation of pH sensitive liposome and evaluate its functionality. **M. Shinohara**, T. Aikawa, T. Kondo, M. Yuasa*
- 856.** Preparation and surface property of fluoroalkyl end-capped oligomer/talc composites: Application to the separation of oil and water. **Y. Oikawa**, T. Saito, S. Yamada, M. Sugiyama, H. Sawada*
- 857.** Preparation and application of fluoroalkyl end-capped vinyltrimethoxysilane oligomer/N-(3-triethoxysilylpropyl)glutamide nanocomposites. **S. Fujii**, T. Saito, H. Sawada*
- 858.** Synthesis of liquid-crystalline organic-inorganic hybrid dendrimers with a magnetite nanocore. **K. Ohsugi**, M. Matsubara, M. Nakaya, A. Muramatsu, K. Kanie*
- 859.** Physical properties of silica nanoparticles coated with mesogenic groups bearing liquid crystallinity and fluorescence. **Y. Ogida**, T. Sanada, K. Kaneko, T. Hanasaki, K. Kojima
- 860.** Development of hydrogel-nanocopper composite and their antibacterial activities against urinary tract infections (UTI) pathogens. **S.M. Asheghi***
- 861.** Highly active and recyclable palladium N-heterocyclic carbene catalyst for Suzuki-Miyaura coupling reaction of unreactive aryl chlorides. **X. Hou***
- 862.** Controllable synthesis of carbon supported metal nanoparticles via ionic liquids-assisted sputtering deposition. **X. GAO**, C. Liu, S. Wang
- 863.** Fabrication technique of the hollow polystyrene nanoparticles by ultraviolet irradiation: Effect of incident angle. **T. Kiryu**, T. Kawai
- 864.** Functional 3D hierarchical assemblies by the *Huisgen-1,3*-dipolar cycloaddition of core-shell nano particles. **S.H. Etschel**, L.F. Portilla, M. Halik, R.R. Tykewski
- 865.** Preparation and structure of calcium hydroxyapatite substituted with light rare earth ions. **A. Yasukawa**, K. Kandori, K. Gotoh
- 866.** Preparation of chitin nanoparticles by regeneration from chitin/ionic liquid solution through high-pressure process. **K. YAMAMOTO**, K. Iimori, J. Kadokawa*
- 867.** Fabrication technique of the hollow nanoparticles by ultraviolet irradiation. **M. TAKAHASHI**, T. Kawai
- 868.** Study on gold nanoparticles-protein interaction by absorbance and fluorescence methods. **X. Qiao**, X. Wu, N. Miyamoto
- 869.** Targeted intracellular protein delivery for cancer therapy. **M. Zhao**, Y. Tang
- 870.** Covalent functionalization of zinc oxide nanoparticles and its photophysical properties. **W. Xiong**, L. Yu, W. Chan, D.L. Phillips
- 871.** Preparation of organic-inorganic hybrid nanoparticles by the miniemulsion system and construction of porous membranes. **H. Takamatsu**, Y. Fukui, K. Fujimoto*
- 872.** Organic-silica hybrid nanomaterials as fluorescent sensors for amines. **D. Sriramulu**, S. Valiyaveettil
- 873.** Preparation of monolithic fluoroalkyl end-capped oligomer/silica nanocomposites for the separation of oil and water. **S. Sasahara**, Y. Aomi, H. Sawada*
- 874.** Surface functionalization and polymer grafting of colloidal silica nanoparticle sol without aggregation of the particles. **T. Maeta**, S. Tamesue, T. Yamauchi, N. Tsubokawa*
- 875.** Preparation and application of fluoroalkyl end-capped vinyltrimethoxysilane oligomer/acrylonitrile-butadiene rubber nanocomposites. **A. Ratcha**, T. Saito, R. Takahashi, S. Kongparakul, H. Sawada*
- 876.** Preparation of xanthan gum nanoparticles through regeneration from ionic liquid solution. **K. Iimori**, D. Hatanaka, K. Yamamoto, J. Kadokawa*
- 877.** Synthesis and characterization of a hybrid magnetic nanosystem for application in thermochemotherapy of cancer. **A. Hervault**, A. Dunn, M. Lim, T. Toshiaki, K. Matsumura, D. Mott, S. Maenosono, T.T. Nguyen
- 878.** Size-selective synthesis of Pd nanoparticles stabilized by dendrimers through stepwise growth method. **H. Hayashi**, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa, K. Kaneda*
- 879.** Enzyme-free electrochemical cholesterol sensor based on NiO/single-layer graphene composite. **G. Lee**, K. Myung, Y. Hu
- 880.** Cancer vaccine using crosslinked CpG oligonucleotide/β-glucans nanoparticles. **N. Miyamoto**, K. Sakurai, S. Mochizuki
- 881.** Synthesis and self-assembly of flexible, free-standing, monolayer gold nanoparticle films. **L. Pruden**, J.S. Shumaker-Parry
- 882.** Site-selective incorporation of nanoparticles into the complex coacervate utilizing self-assembly of block copolymers in aqueous solution. **K. Naoyama**, T. Mori, Y. Katayama, A. Kishimura*

Hawaii Convention Center
Halls I, II, III

Nanocrystal Synthesis, Characterization, Assembly and Applications (#34)

Organized by: R. Tilley, S. Skrabalak, T. Hyeon, T. Nann, T. Adshiri

Poster Session

10:00 – 12:00

- 883.** Blue inorganic light emitting diode on flexible polyimide substrate using laser lift-off process. **N. Barange**, Y. Kim, I. Han, D. Ko
- 884.** Bio-fabrication of nanoporous gold membrane with anti-inorganic bispecific nanobody. **T. Niide**, H. Nakazawa, I. Kumagai, M. Umetsu*, N. Manabe
- 885.** Self-assembling of gold nanoparticles on ionic liquid surface via ionic liquid-metal sputtering. **D. Sugioka**, T. Kameyama, S. Kuwabata, T. Torimoto*

* Principle Author

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<http://pacifichem.org/onlineprogram>

- 886.** Facile preparation of aramid and polybenzoxazole nanofibers from synthetic fibers by a downsizing process. **S. Ifuku***, H. Maeta
- 887.** Surface-enhanced Raman scattering measurements using a tunable plasmonic device on hydrogels. **H. Mitomo***, K. Horie, Y. Matsuo, K. Niikura, T. TANI, M. Naya, K. Ijiro
- 888.** Synthesis and characterizations of SnO₂ nanorods using low temperature hydrothermal technique. **H. Lee***, S. Lim, V. Inderan
- 889.** Enhanced of catalytic performances over skeletal Ni catalysts prepared from heated Ni-Zr amorphous alloys in various structural states and composition. **Y. Tanihara**, A. Nozaki, Y. Kuwahara, T. Ohmichi, K. Mori, H. Yamashita*
- 890.** Synthesis of lithium metal phosphates and silicates for Li-ion battery. **Q. TRUONG**, I. Honma
- 891.** Active skeletal Au catalysts prepared from Au-Zr amorphous alloy. **A. Nozaki**, Y. Tanihara, Y. Kuwahara, T. Ohmichi, K. Mori, H. Yamashita*
- 892.** PdRu solid-solution nanoparticles: Size-controllable synthesis and size-dependent catalytic properties. **D. Wu***, K. Kusada, H. Kitagawa
- 893.** Photocatalytic performance of nanostructured porous silica and TiO₂ composites in environmental purification. **Y. Ishiguro**, T. Kamegawa, H. Yamashita*
- 894.** Mechanistic study of precursor conversions at low temperature to binary colloidal nanocrystals. **K. Yu***
- 895.** Microwave assisted synthesis and characterization of MgO nano structures in structural directing monocationic and dicationic ionic liquids and nano structures catalytic activity in organic transformation. **A. Jadhav***, G. Thorat, J. Seo*
- 896.** Design on yolk-shell nanostructures for efficient lithium ion storage. **S. Guo**
- 897.** Size minimization of BaHfO₃ flux pinning centers in YBa₂Cu₃O_y superconducting films by chemical solution deposition process. **R. Teranishi***, H. Horita, K. Ootaguro, K. Yamada, K. Kaneko, M. Yoshizumi, T. Izumi
- 898.** Structural characterisation of multimetallic nanoparticles using XAS. **I.J. Godfrey**, A. Dent, I.P. Parkin, S. Maenosono, G. Sankar*
- 899.** Growth, structure, and optoelectronic properties of crystalline binary pyrophosphates. **U. Mazur**, K. Hipp
- 900.** Using nuclear magnetic resonance (NMR) techniques to study small ($d = 2\text{--}3$ nm) gold-transition metal nanoparticle alloys. **L. Marbella**, C. Andolina, J.E. Millstone
- 901.** Facile synthesis of composition-gradient Cd_{1-x}Zn_xS quantum dots by cation exchange for controlled optical properties. **D. Choi**, J. Pyo, Y. Kim, **D. Jang**
- 902.** Synthesis of Au-Pt composite nanoparticles with controlled composition ratio by solution plasma processing. **T. Chiyoda***, M. Banjo, H. Yui
- 903.** Self-assembly of photonic crystal of silver-based nanoparticles and double-effect on fluorescent enhancement. **F. Ge***
- 904.** Synthesis, characterization, and formation mechanism of Mn₃O₄ hollow microspheres. **Q. Li**, C. Jiang*, W. Zhou*
- 905.** Hydrothermal growth of yttria-stabilized zirconia nanocrystals aqueous dispersions. **N. Pouy***, K. Sato*, K. Horiguchi, H. Abe
- 906.** Metal nanoparticle synthesis using poly(ethylene oxide)-poly(propylene oxide) block copolymers in aqueous media. **A. Ishihara**, T. Sakai, P. Alexandridis
- 907.** Metal nanoparticle deposition on silica spheres using poly(ethylene oxide)-poly(propylene oxide) block copolymers in solutions. **T. Watanabe***, T. Sakai, P. Alexandridis
- 908.** Photocurrent enhancement of colloidal quantum dots solar cell by surface treatment. **R.O. Ferreira***, S. Masuo
- 909.** Self-assembly of gold nanoparticles into vesicle-like structures by the use of a carbohydrate-terminated fluorinated surface ligand. **J. Wei**, N. Sugimura, K. Niikura, H. Mitomo, K. Ijiro
- 910.** Preparation and physical properties of nanoaggregates composed of organic dyes with a D-π-A structure. **M. Imai**, S. Okada*
- 911.** Synthesis of BaTaO₃ photocatalyst by ammonothermal method. **T. Toshima**, K. Kishida, T. Watanabe
- 912.** Continuous reactive crystallization of GZO particles in supercritical water and formation mechanism. **K. Sugawara**, T. Sato, M. Matsumoto, M. OKADA, T. Hiaki
- 913.** Fabrication of PbS colloidal quantum dot solar cell: Relationship between photovoltaic performance and surface modification. **N. Tsuji***, S. Masuo
- 914.** Direct synthesis of liquid metal colloids and their transformation into metal oxide nanoparticles. **S. Sudo**, K. Kokado*, K. Sada*
- 915.** Liquid phase synthesis of Bi₂Te₃ nanoparticles for thermoelectric transducer. **Y. Shibuya***, M. Nakaya, A. Muramatsu, Y. Kinoshita, M. Ishikiriyama
- 916.** Tuning of the gap-mode plasmon band of silver nanoparticle films by controlling of the silver nanoparticle size. **T. Togashi**, S. Soma, K. Kanaizuka, M. Kurihara
- 917.** Formation of Pd nanocrystals from Pd₂(dba)₃ microcrystals. **S. Chung***, D.N. Leonard, V. Altoo, S. Aloni, J.J. De Yoreo, S. Franzen
- 918.** Solution phase synthesis of near-infrared light-responsive quantum dots comprised of ZnTe-AgInTe₂ solid solution. **K. Sugura**, T. Kameyama, S. Kuwabata, T. Torimoto*
- 919.** Carrier dynamics of trion in CdSe nanocrystals by photochemical electronic doping. **N. Kakimoto**, Y. Usui, T. Okuhata, N. Tamai
- 920.** Effects of cross-linking structure by alkane diethiol for stability and conductivity of 2D silver nanoparticle sheets. **N. Saito**, S. Ryuzaki, K. Okamoto, K. TAMADA*
- 921.** Synthesis of some crystal forms of Ce-Zr composite oxide by freeze-sintering method. **T. Kohirulaimaki***, S. Yoshida
- 922.** Low temperature solid state synthesis of metallic magnetic nanoparticle loaded to multiwalled carbon nanotubes. **L. Steinberg***, S. Yamamoto, Y. Kobayashi, H. Kageyama
- 923.** Stabilization of the superionic phase of AgI nanoparticles to room temperature under high pressure. **T. Yamamoto***, M. Maeato, Y. Asakawa, G. Kawaguchi, Y. Ohishi, N. Hirota, H. Kobayashi, H. Kitagawa
- 924.** Mechanistic insight into the Yolk@Shell transformation of MnO@Silica nanospheres incorporating Ni²⁺ ions toward a colloidal hollow nanoreactor. **J. Kim***, I. Lee*
- 925.** Synthesis and optoelectronic applications of branched semiconductor nanocrystals. **N. Mishra**, Y. CHAN, J. Hollingsworth
- 926.** Hydrothermal growth of tailored SnO₂ nanocrystals. **y. motegi**, K. Sato*, Y. Yokoyama, V. Jean-Christophe, H. Abe
- 927.** Surface capping-assisted hydrothermal growth of gadolinium-doped CeO₂ nanocrystals. **K. Sato***, M. Arai, V. Jean-Christophe, H. Abe
- 928.** Surface-specific deposition of catalytic metal nanocrystals on hollow carbon nanospheres via galvanic replacement reactions of carbon-encapsulated MnO nanoparticles. **D. Lee**, S. Kim, I. Lee*
- 929.** Synthesis and properties of quantum-sized metal oxide clusters by using dendrimer as a template. **Y. Inomata**, K. Albrecht, K. Yamamoto
- 930.** Investigation of the factor for controlling C₆₀ nanocrystal structure. **N. Ito**, K. Shito, A. Masuhara
- 931.** Subnanometric PtO_x clusters deposited on CeO₂ nanowires for low-temperature CO oxidation. **J. Ke***, W. Zhu, Y. Jiang, R. Si, C. Jin, H. Liu, C. Yan, Y. Zhang
- 932.** Electrochemical decomposition of borosilicates made from kerf loss silicon and deposition of crystalline silicon. **K. Tomono***, R. Sakamoto, M. Okada, S. Kakihara, Y. Tamaki, Y. Yahata
- 933.** Principle of anisotropy in biomineralization: Anisotropic mineral growth in elongated hydrogel. **K. Fukao**, T. Nonoyama, K. Furusawa, T. KUROKAWA, T. Nakajima, J. Gong*
- 934.** Controlling perovskite crystal size and its thin film. **Y. Hayasaka**, K. Umemoto, A. Masuhara
- 935.** Synthesis and characterization of semiconducting copper manganese sulfide nanoparticles. **K. Gupta**, M.S. Singh, D. Mott, S. Maenosono*
- 936.** Organic-organic hybridized nanocrystals using reprecipitation method and oxidative polymerization. **H. Watanabe***, T. ARITA, K. Miyakawa, A. Masuhara
- 937.** Nanocrystallization processes of C₆₀ in the reprecipitation method. **K. Shito***, N. Ito, T. Iino, A. Masuhara
- 938.** CH₃NH₃PbI₃(methyl ammonium lead tri-iodide) perovskite film prepared by colloidal deposition technique. **K. Umemoto***, Y. Hayasaka, A. Masuhara
- 939.** Au-SiO₂-P3HT core-shell type nanoparticles for plasmonic organic photovoltaic devices. **K. Miyakawa**, H. Watanabe, H. Naiki, H. Uji, T. ARITA, A. Masuhara
- 940.** p-type Co₃O₄/ZnCo₂O hollow sphere: High performance formaldehyde detection at ppb levels. **J. Kim***, H. Park*, D. Lee, H. Song
- 941.** Surfactant-assisted shape evolution of 3D molecular architecture. **M. Jeon**, S. Kwon, H. Lee*
- 942.** Induction of thermoresponsive behavior in gold nanoparticles by the display of low molecular weight surface ligands. **R. Iida***, K. Niikura, H. Mitomo, K. Ijiro
- 943.** Green synthesis of Cu/Cu₂O core/shell nanoparticles with lowered resistivity. **S. Yokoyama***, K. Motomiya, H. Takahashi, K. Tohji
- 944.** Experimental and theoretical investigation on the formation of platinum decorated nickel nanocubes. **A. Nagao***, T. Ishimoto, M. Koyama, H. Miyamura, J. Cuya, J. Balachandran
- 945.** Dispersion dependent stability and catalytic activity of hybrid Fe₃O₄/Pd catalysts in water for suzuki coupling reactions. **D. Kim**, H. Woo, K. Park
- 946.** C₆₀ nanocrystals thin film by liquid-liquid interface assembly technique. **S. Morizane***, M. Takeda, J. Matsui, A. Masuhara
- 947.** Organic nanocrystals and these layered structure for organic solar cells. **A. Masuhara***, K. Shito, S. Morizane, A. Ito, K. Nakayama, T. Yoshida, J. Matsui
- 948.** Preparation and characterization of TiO₂ anchored silica fibers derived from titanium alkoxy-dilopate precursor. **A. Hasegawa***, M. Ekari, T. Honma
- 949.** High performance electrochemical capacitors composed of mesoporous manganese dioxide and fullerene C₆₀ nanocrystals. **A. Toba***, Y. Matsukubo, A. Masuhara
- 950.** Hydrothermally synthesized CeO₂-CuO composites as a catalyst for CO oxidation. **M. guo**, F. Liu, J. Tsui, **A. Ng**, A. Djurišić, W. Chan

9:20 – 954. Semiconductor nanowire array grown by selective area epitaxy and their applications. **T. Fukui**

9:50 Break

10:00 – 955. Integrated Group IV nanowire optoelectronics. **M. Jo***

10:30 – 956. Synthesis and optoelectronic properties of pseudobinary solid-solution semiconductor nanowires. **B. Liu***, X. Jiang

11:00 – 957. Band gap-engineering within single semiconductor nanostructures. **A. Pan**

11:30 – 958. Unusual nanoscale electronic effects in heterojunction nanowires. **B.M. Wong***

11:45 – 959. Manipulating the optical and electrical properties of a single ZnO nanowire through interfacial modulation doping. **N. PAN***, H. Ding, Y. Wu, C. Ma, Y. Luo, X. Wang

Hawaii Convention Center
318A

Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95)

Organized by: J. Kawamata, J. Choy, C. Lee, D. Tellier, H. Zhang, J. Huang, L. Wan
Presiding: J. Huang, H. Zhang

8:00 Break

8:30 – 960. Molybdenum disulfide as a highly efficient absorbent for nonpolar gases. **L. Wang**

8:50 – 961. Growth and characterization of single-layer MoS_{2(1-x)Se_x} alloy films. V. Klee, D. Barroso, Q. Ma, J. Mann, L. Bartels

9:10 – 962. 2D materials: From doped monolayers and defects to van der Waals solids and more. **M. Terrones**

9:40 – 963. 2D layered materials, heterostructures, and devices. **X. Duan**

10:10 Break

10:30 – 964. Atomic layer deposition of 2D MoS₂ on 150nm Si/SiO₂ substrates. A. Valdivia, **J. Conley**

10:50 – 965. Regulating electrical properties of inorganic 2D nanomaterials for energy storage and electrocatalytic applications. **C. Wu***

11:10 – 966. Hydrogen storage in Ni/graphene and Pd/graphene composites. C. ZHOU, **J. Szpunar**, J. Wang, Y. Hu

11:30 – 967. Heterostructures based on CVD transition metal dichalcogenides. **L. Li**

Hawaii Convention Center
321B

Applications of Ultrasound to Nanoscience (#150)

Organized by: K. Suslick, F. Grieser, M. Atobe, J. Yu, S. Jeong
Presiding: J. Yu

8:00 – 968. Utilization of nanostructured materials for stem cell applications. **W.H. Suh***

8:30 – 969. Sonochemical treatment of surfaces for optimized cellular interaction. **H. Moehwald**, V. Belova-Magri, E.V. Skorb

* Principle Author

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9:00 – 970. Sonochemically produced nanomaterials for combatting dental disease.
G.J. Price

9:30 – 971. Sonochemical sample preparation for biological assays. **T. Matula***, K. Bomsztyk, B. MacConaghay, A. Maxwell

10:00 – 972. Polydopamine based perfluorocarbon nanodroplets for medical ultrasound applications. **B. Teo**, J.Y. Lee, A. Seth, E. Stride

10:30 Coffee and Bio Break

10:40 – 973. Preparation of polymeric ultrasonic/MRI dual mode contrast agent and its responsive drug release capacity.
F. Yang*

11:00 – 974. Sonochemical synthesis and characterization of polysaccharide-shelled microspheres. **M. Zhou***, Q. Ye, M. Ashokkumar

11:20 – 975. Numerical study on nucleation and oriented aggregation of BaTiO₃ nanocrystals. **K. Yasui***, K. Kato

Hawaii Convention Center
Halls I, II, III

Mechanically Responsive Materials (#153)

Organized by: P. Naumov, T. White, B. Kahr, Y. Yu

Poster Session

10:00 – 12:00

976. Shear-piezoelectric properties of Poly(L-lactic acid) woven fabric based sensors for monitoring human respiration pattern. **Y. Ahn**, E. Song, A. Prabu, K. Kim*

977. Highly sensitive paper-based pressure sensors. K. Lee, **w. shim***

978. Photomechanical bending of chiral and racemic crystals of azobenzene derivatives. **T. Taniguchi**, M. Shiro, H. Koshiba*, T. ASAHI

979. Route for systematic preparation of photomechanical azobenzene cocrystals. **O. Bushuyev***, A. Tomberg, T. Friscic, C. Barrett

980. Photomechanical performance of dialeythene single crystals. **M. Morimoto***

981. Bending behavior analysis of silicone elastomer film. **Y. Koike**, N. Nakamatsu, S. Fujikawa, A. Shishido*

982. Development of mechanical analysis system of flexible films. **N. Akamatsu**, S. Fujikawa, A. Shishido*

983. Piezoelectricity of nanowires via electrospinning optical isomers of Poly(lactic acid) and their racemic mixture. **K. Kim***, E. Song, A. Prabu, Y. Ahn

Hawaii Convention Center
322AB

Current and Future Applications of Nanotechnology in the Oil Industry (#197)

Organized by: W. Wang, K. Lee, J. Ordóñez-Varela, M. Kanj, T. Jiang
Presiding: W. Wang

8:00 opening remark

8:05 – 984. "NanoProbes" for reservoir surveillance and recovery. **M.E. Poitzsch***

8:35 – 985. Iron-oxide and silica nanoparticles with specific surface coatings for upstream oil & gas applications. **C. Huh***

9:05 – 986. Exploration of rare earths based luminescence for detection and sensing in radiation security and enhanced oil recovery. **W. Chen***

9:35 break

9:50 – 987. Shale gas fracturing fluids using polymer grafted silica with enhanced suspending. M. Bell, A. Viswanath, **B.C. Benicewicz***

10:15 – 988. Hybrid ionic-nano additives for advanced lubrication. **J. Qu***

10:40 – 989. Investigation of a kind of complex oil displacing method containing micro-nano microspheres after polymer flooding. **H. Yang**, **W. Kang**, Y. Yu, Y. Lu, Z. Li

Hawaii Convention Center
320 Theatre

Frontiers of Organic Porous Materials: Structures, Properties and Applications (#223)

Organized by: D. Jiang, W. Wang, W. Zhang
Presiding: P.M. Budd, J. Zhang

8:00 – 990. π-Conjugated porous organic frameworks as photoredox catalysts. **J. Zhang***

8:25 – 991. Computer aided design of micro-porous organic polymers for the energy applications. **W. Deng***, L. Sun, Y. Xie
8:50 – 992. Gas storage and separation-directed design and synthesis of porous aromatic frameworks. **G. Zhu**

9:15 – 993. Slipping induced variation in CO₂ and CH₄ adsorption and selectivity in various covalent organic frameworks. **R. Babarao***, A. Sharma, N. Medhekar, A. malani

9:30 – 994. Imine-based organic porous materials: From single molecule to extended framework. **C. Wang***, H. Ding, H. Liao

9:45 Coffee Break

9:55 – 995. Polymers of intrinsic microporosity (PIMs): Tailoring selectivity through chemical modification. **P.M. Budd***

10:20 – 996. Graphitic carbon nitride polymers for solar water splitting. **x. wang**

10:45 – 997. Task-specific functionalization of porous organic polymers. **S. Ma***

11:10 – 998. Liquids with permanent micro-porosity - a new phase for porous materials. **S. James**

11:25 – 999. Diversity of covalent organic frameworks (COFs): From single-pore to dual-pore. **X. Zhao***

11:40 – 1000. Rotor dynamics and photo-induced porosity switch in supramolecular architectures and covalent frameworks. **P. Sozzani***, S. Bracco, A. Comotti

11:55 Closing Remark

Hawaii Convention Center
319A

Self-organization of Membrane Systems (#259)

Organized by: D. Sasaki, K. Morigaki, I. Kooper
Presiding: K. Morigaki

8:00 – 1001. Creating lipid bilayer platforms insensitive to air-water interfaces by physical confinement. **L. Chao***, C. Han

8:30 – 1002. Designed amphiphilic polymers for lipid membrane nanodisc formation. **K. Yasuhara***, J. Arakida, J. Kikuchi

8:50 – 1003. How to manipulate self-organization of lipid components for RAFT formation by topographic curvature in model membrane. **S. Lee***, Y. Ryu

9:20 – 1004. On-chip lipid microfluidics: Controlled self-organize to form biomembranes. **N. Cho***

9:40 Break

9:50 – 1005. Microfluidic technology for artificial lipid bilayer formation. **S. Takeuchi**

10:20 – 1006. Fundamental studies of osmotic transport across the droplet lipid membrane: Lipid structure, asymmetry, and cholesterol. **S. Lee***

10:40 – 1007. Single molecule transporter assay with arrayed lipid bilayer chamber systems. **H. Noji***

11:10 – 1008. Artificial membranes composed of fluid and polymerized lipids: Assembly, structure, and application to receptor-based biosensing. **S. Saavedra**

11:30 – 1009. Nanopores with fluid lipid membrane coatings for characterization of single proteins in solution. **M. Mayer**

Hawaii Convention Center
318B

Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308)

Organized by: R. Morandotti, D. Moss, F. Omenetto, N. Tsutsumi, K. Alamgir, K. Char, A. Faccetti
Presiding: A. Karim

8:00 – 1010. Nanomembrane materials and soft fabrication methods for high performance photovoltaic systems: Low cost, full spectrum solar energy conversion. **R.G. Nuzzo***

8:30 – 1011. Fluctuations and cooperative motion in the interfacial dynamics of nanoparticles. **J.F. Douglas**, H. Zhang

9:00 – 1012. Preparation of new photoactive materials: From a proof-of-concept to functional materials. **A. Laventure**, D. Lauzon, J. Bourotte, J. Väpäavuori, R. Sabat, O. Lebel, C. Bazulin, C. Pellerin*

9:20 – 1013. Design of full-color thermally activated delayed fluorescence emitters based on benzonitrile derivatives and their application in organic light-emitting diodes. **I. Park**, T. Yasuda*, S. Lee, C. Adachi*

9:40 – 1014. Physical and electrochemical reconciliation of Cu₂ZnSnS₄ thin film absorber properties. **D. Vaccarello**, Z. Ding*

10:00 Break

10:10 – 1015. Slot-die processing of PTB7/PC₇₁BM: Understanding morphology evolution and device performance. **T.P. Russell***, S. Ferdous, C. Wang, E. Schaible, A. Hexemer

10:40 – 1016. Controlling molecular weight of conjugated polymers as a powerful tool for optimizing the efficiency of all-polymer solar cells. **A. Dudnik**, N. Zhou, T.J. Aldrich, T. Li, E.F. Manley, Z. Chen, R.P. Chang*, L.X. Chen*, M. Olvera de la Cruz*, A. Faccetti*, T.J. Marks*

11:00 – 1017. Novel oxide thin-film diode for oxide electronics. **J. LEE**, E. Lee, J. Park, Y. Kim*

11:20 – 1018. Structural diversity in donor-acceptor materials - adducts of trimeric perfluoro-o-phenylene mercury. **T.V. Timofeeva***, R. Castaneda, M. Fonari, Y. Getmanenko

11:40 – 1019. Novel phosphorescent complexes with bipolar charge-transporting ability for highly efficient organic light-emitting diodes (OLEDs). **Y. Liu***, J. Feng*

Hawaii Convention Center
319B

Membranes and Nanotechnologies for Energy and Environment Applications (#317)

Organized by: H. Park, B. Freeman, B. McCloskey, J. McGrath, A. Hill, A. Higuchi, Y. Lee

8:00 – 1020. Polymeric membranes for CO₂ separation. **H. Lin***, L. Zhu, J. Liu, B. Lam

8:30 – 1021. Interplay between CO₂ separation properties and membrane morphology. **I. Taniguchi***, K. Kinugasa

8:50 – 1022. Ultrathin composite membranes for CO₂ separations. **G.G. Qiao**

9:10 – 1023. 6000 GPU poly(ionic liquid)/ionic liquid composite membrane for CO₂/N₂ separations. **M.G. Cowan**, J. Zhou, M.M. Mok, W. McDowell, T.K. Carlisle, D. Gin, R.D. Noble

9:30 – 1024. Mixed CO₂/CH₄ sorption in PIM-based membranes. A. Gameda, **M. De Angelis**, G.C. Sarti, M.D. Guiver

9:50 – 1025. Molecular separation by a free-standing and nanometer-thick membrane. **S. Fujikawa***

10:20 – 1026. Effect of water vapour on CO₂ separation performance mixed matrix membranes. **S. Kaneshashi***, G.Q. Chen, C.A. Scholes, S.E. Kentish

10:40 – 1027. Polymer supported metal-organic framework nanocomposite hollow fiber membranes for gas separation. **J. Hou**, P. Sutrisna, H. Li, Y. Zhang, **V. Chen***

11:00 – 1028. Formation of CHA zeolite membranes by secondary growth for post-combustion carbon capture. **E. Kim**, **J. Choi***

11:20 – 1029. Novel ionic group-mediated crosslinked polyimide membranes for high performance CO₂ separation. **T. Kim***

Hawaii Convention Center
316C

Ceramic Materials and Processing for Advanced Applications (#341)

Organized by: F. Rosei, A. Vomiero, Y. Tachibana, C. Raston, H. Zhang

8:00 – 1030. Ultrafast transmission electron microscopy and its nanoplasmatic applications. **A. Yurtsever***

8:30 – 1031. Solution-based bioinspired growth of photocatalytically active nanoporous membranes, and oriented nanowires for water purification and splitting. **D. Kisailus***

9:00 – 1032. Ultrafast spectroscopic study of trapped state sensitive kinetics in LaTiO₃N solid photocatalysts. **A. Furube**, R. Singh, H. Matsuzaki, Y. Suzuki, K. Seki, T. Minegishi, T. Hisatomi, K. Domen

9:20 – 1033. Synthesis optimisation of mesoporous Ti-silica microspheres for efficient oxidative and photocatalytic applications. **A.S. Perera**, M. Coppers*

9:40 coffee break

10:00 – 1034. Near-infrared excited lanthanide-doped nanoparticles with core/shell architectures for theranostic applications. **F. Vetrone***

10:30 – 1035. Electron-transfer mechanism of dye-sensitized solar cells with high performance hydrotalcite nano clay electrolytes. **S. Uchida***, D. Sakurai, T. Kubo, H. Segawa

11:00 – 1036. Rare-earth-ions-doped calcium chlorapatite phosphors: Synthesis, structures, and photophysical characterization. **K. Hong***, M. Ha, B. Kang, H. Kim, H. Yang

11:20 – 1037. Tunable phase and coloration of iron based ceramic nano pigments. **Y. Kim***, R. Yu

11:40 – 1038. Novel environmentally friendly red pigments based on orthorhombic bis-muth vanadate. **D. WEN**, S. Tamura, T. Masui, N. IMANAKA*

Hawaii Convention Center
316B

Materials for the Mitigation of Chemical Hazards (#388)

Organized by: J. DeCoste, G. Peterson, J. Becker, M. Biggs, L. Croll, K. Walton
Presiding: J. DeCoste

8:00 – 1039. Screening of functionalized or hydrophobic MOFs for capture of ammonia and other toxic compounds. **P.Z. Moghadam**, K. Kim, Y. Zeng, P. Ghosh, D.J. Fairén-Jimenez, **R.Q. Snurr***

* Principle Author

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8:30 – 1040. Highly efficient photocatalytic activity by five-layer Aurivillius phase perovskites under solar irradiation.
T.K. Mandal*, N. Gollapally

8:50 – 1041. New multifunctional POM-containing materials for decontamination and protection. **C.L. Hill***, W. Guo, K. Sullivan, H. Lv, Z. Luo, N. Pomerantz

9:20 – 1042. Nerve agent degradation with polyoxoniobates. **M. Nyman**

9:40 – 1043. Chemical sensing and destruction of hazardous chemicals using metal oxides and hydroxides. **J.E. Whitten***

10:10 Break

10:20 – 1044. Metal–organic frameworks as highly functional catalytic arrays. **O.K. Farha***

10:50 – 1045. Tailoring the nucleophilic character of metal-organic frameworks for the reactive removal of chemical threats. **J. DeCote***, M.A. Browne, G.W. Wagner, G. Peterson

Hawaii Convention Center
314

Design of Innovative Photochromic Applications (#399)

Organized by: J. Abe, T. Kawai, Y. Yokoyama, N. Branda, F. Raymo, W. Zhu

Presiding: J. Abe

8:00 Opening

8:05 – 1046. Using photochromes to mimic photosynthetic photoregulatory processes. **D. Gust***, T.A. Moore, A.L. Moore

8:25 – 1047. Elucidation and control of photochromic reactions by pulsed laser excitation. **H. Miyasaka**

8:45 – 1048. On the design of efficient photochromic system. **S. Hecht***

9:05 – 1049. Photo-active energetic materials. **R.J. Scharff***

9:25 – 1050. Revealing transient species of photochromic phenoxy-imidazolyl radical complexes by time-resolved infrared absorption spectroscopy. **Y. Kobayashi**, H. Yamashita, S. Toshimitsu, J. Abe*

9:45 Break

10:00 – 1051. Dynamics and isomerization in photochromic ruthenium sulfoxide complexes. **J. Rack**, A. King

10:20 – 1052. Oxazolidines: Trimodal switchable units and molecular tango. **J. pozzo**

10:40 – 1053. Stepwise photochromism triggered by metal coordination in multidiethylenethene (DTE) systems. **Z. Chen***

11:00 – 1054. Benzobis(thiadiazole)-based diarylethenes: Sterical hindrance offering full separation of conformers with chiral resolution. **W. Zhu***

11:20 – 1055. Synthesis, photochemistry, electrochemistry, and computation: Toward functional “photochromic photooxidants”. **J.G. Gillmore**

11:40 – 1056. Spiropyran-cyclodextrin coated metal oxide nanoparticles for photochromic light-harvesting applications. **V. Dryza***, E. Bieske

Hawaii Convention Center
Halls I, II, III

Single-Molecule Function and Measurements (#408)

Organized by: T. Ogawa, H. Tada, S. Park, P. Weiss

Poster Session

10:00 – 12:00

1057. Synthesis and conductance measurement of single molecular slide switch. **T. TAMAKI**, R. Yamada, H. Tada, T. Ogawa*

1058. Synthesis and physical properties of a porphyrin Tb dinuclear complex designed for spintronics. **N. Sakata**, S. Lee, N. Sumitani, T. Inose, R. Yamada, H. Tada, D. Tanaka, T. Ogawa*

1059. Synthesis of polycyclic aromatic hydrocarbons by AuCl catalyzed multicyclization: Candidates for a rigid π organic molecular junction. **T. Nakae***, S. SATO, M. Takase, S. Mori, T. Okujima, H. Uno, H. Sakaguchi

1060. Synthesis, properties, and electrical conductance of insulated oligothiophenes having spiro-substituted fluorenes. **Y. Okamoto**, Y. Ie, R. Yamada, S.K. Lee, H. Tada, Y. Asao

1061. Single molecule electronic properties of perpendicularly connected porphyrin-imide dyads. **Z. Chen**, M. Handayani, R. Yamada, H. Tada, H. Tanaka, T. Ogawa*

1062. Synthesis and physical properties of cyclo[8]porphyrrole-polyoxometalate complex. **H. Matsumoto***, F. Miyamoto, Y. Yamazaki, T. Ogawa, S. Mori, M. Takase, H. Uno, T. Okujima

1063. Synthesis of cyclic-insulated conjugated anchor molecule and its immobilization on ITO substrate. **H. Masai**, S. Kaneko, J. Terao, T. Katase, H. Ohta, T. Fujihara, Y. Tsuji

1064. Programming the potential gradient of phenylazomethine dendrimer. **K. Albrecht**, K. Yamamoto*

1065. Synthesis and properties of bisporphyrin connected by chrysene-like bridge with two bicyclic skeletons. **S. Mori**, N. Kawamoto, T. Okujima, H. Uno*

1066. Multidimensional mixed-valence complex with a Ni porphyrin linker. **Y. Tanaka**, K. Mishiba, M. Akita*

1067. Single molecule devices connecting to three carbon nanotube electrodes. **A.Y. Akbar***, M. Handayani, A.I. Abd El-Mageed, T. Ogawa

1068. Fabrication and electric properties of graphene nanoribbons obtained by SWNT. **M. Fukumori***, H. Tanaka, T. Ogawa

1069. Synthesis of insulated molecular wires containing transition metals in their backbones. **T. Hosomi**, H. Masai, W. Matsuda, J. Terao, S. Seki, T. Fujihara, Y. Tsuji

1070. Fabrication and electrical properties of X- and Y- structures of unzipped single-layer graphene nanoribbons. **P. Liu**, S. Kasai, X. Yin, T.K. Yamada, T. Ogawa, M. Fukumori, H. Tanaka*

1071. Edge structure controlled synthesis of graphene nanoribbons by radical polymerization-chemical vapor deposition. **S. Song**, T. Nakae, T. Kojima, H. Sakaguchi*

1072. Nanoscale charge transport of DNA supramolecular networks. **H. Yamaguchi***, D. Che, T. Matsumoto

1073. Electrical detection of single DNA molecules by electrode-embedded nanopore devices. **K. Yokota***, M. Tsutsui, T. Ohshiro, M. Taniguchi, T. Kawai

1074. Two-step tunneling conduction through a single cytochrome c₃ molecule. **S. Sumida***, D. Che, T. Matsumoto

1075. Environmental control of single-molecule conductance. **H. Okuyama**

1076. Imaging of electrostatic potential in organic photovoltaic thin film. **K. Araki***, Y. Ie, Y. Asao, T. Matsumoto

1077. Structure controlled construction of metal-porphyrin molecular layers by self-assembly technique. **N. Aoki**, Y. Ishikawa, A. Shokai, M. Hase, T. Kondo*

1078. Formative mechanism of single-molecule junctions. **S. Tanimoto**, T. Morikawa*, A. Arima, M. Tsutsui*, M. Taniguchi*

1079. First-principles simulations of the switching mechanism in tantalum oxide-based resistive memory devices. **A. Nakayama***, J. Hasegawa, H. Nakamura*

1080. Direct quantitative analysis of HCV RNA by atomic force microscopy without labeling or amplification. **Y. Jung***

1081. Design of nano-electronic neural-network associative memory circuit for single-molecule devices. **M. Takano***, T. Asai, T. Oya

1082. Design of new logic circuit mimicking soldier crab ball gate for single-molecule device. **Y. Hamana***, T. Asai, T. Oya

1083. Design of thermal-noise-harnessing neuromorphic nano-electronic circuit based on axon of neuron for single-molecule device. **R. Hirashima***, T. Asai, T. Oya

1084. Amoeba-inspired computing system utilizing charge dynamics in a capacitor network with spatiotemporal fluctuation. **R. Wakamiya**, S. Kasai, M. Aono, M. Naruse, M. Hiroyoshi

1085. Design of single-electron “slime mold” circuit for single-molecule device. **K. Satomi***, T. Asai, T. Oya

1086. Chaotic analysis of neuron-firing reproducing device of POM/CNT random network. **F. Lingxiang**, H. Tanaka*, H. Tamukoh, T. Ogawa

Hawaii Convention Center
315

Advances in Organic Light-Emitting Diodes (#409)

Organized by: J. Bredas, C. Adachi, K. Wong, V. Yam, P. Burn, J. Kim

Presiding: P.L. Burn

8:00 – 1087. Advances in quantum dot spectroscopy and applications. **M. Bawendi***

8:30 – 1088. Molecular triplet emitters - from design to assembly and functions. **V. Yam**

8:50 – 1089. Power efficient solution-processed white organic light-emitting diodes with ultra-high color stability. **L. Wang***

9:10 – 1090. TADF combined with short-lived phosphorescence: Novel concept for OLED emitters based on Cu(I) complexes. **K.M. Takeda***, K. Osada, T.A. Tockary, Q. Chen, A. Dirisala, K. Kataoka

9:30 – 1091. Latest progress and its fundamentals for polymer-OLED material development. **T. Yamada**

10:00 Break

10:20 – 1092. Device architecture for highly efficient flexible organic light-emitting diodes (OLEDs). **S. Yoo***, E. Kim, J. Lee, J. Song

10:50 – 1093. Thermally activated delayed fluorescence in isometrically designed donor-acceptor mixed-stacked charge-transfer cocystal. **S. Park**, J. Gierschner, S. Park*

11:10 – 1094. Electroluminescence generated through spin-independent band recombination and spin-dependent molecular recombination regimes in organic-inorganic halide perovskites. **B. Hu***

11:30 – 1095. Current status and future of OLED lighting. **S. Park**

Hawaii Convention Center
317B

The Frontiers of Geometrically Frustrated Magnetic Materials (#430)

Organized by: C. Wiebe, C. Ling, J. Gardner, H. Zhou

8:00 – 1096. Frustration under pressure: exotic magnetism in new pyrochlore oxides. **C. Wiebe***

8:40 – 1097. High-pressure syntheses and characterizations of the rare-earth germanate pyrochlores R₂Ge₂O₇. **J. Cheng**, X. Li, Z. Dun, A.M. Hallas, h. zhou, C. Wiebe

9:20 – 1098. Incipient ferromagnetism in Tb₂Ge₂O₇: Application of chemical pressure to the enigmatic spin-liquid Tb₂Ti₂O₇. **A. Hallas***, A. Arevalo-Lopez, J.P. Attfield, J. Cheng, h. zhou, G. Luke, C. Wiebe

9:35 – 1099. Quadrupole order and spin liquid state of Tb_{2+x}Ti_{2-x}O_{7+y}. **H. Kadokawa**

10:15 Coffee Break

10:25 – 1100. Spin liquids in two new pyrochlore materials. **R. SIBILLE***, T. FENNEL, E. LHOSTEL, M. Ciomaga Hatnean, G. Balakrishnan, M. KENZELMANN

10:40 – 1101. Elastic anomalies in orbital-degenerate frustrated spinel Co₂O₄. **T. Watanabe***, S. Yamada, R. Koborinai, T. Katsufuji

11:20 – 1102. Strong competition between orbital ordering and itinerancy in a frustrated spinel vanadate. **h. zhou**

Hawaii Convention Center
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Self-assembled Biofunctional Nanomaterials (#433)

Organized by: R. Nagarajan, K. Sakurai, H. Chen

Poster Session

10:00 – 12:00

1103. Coating of electrodes with self-organized HFBI membrane: Structure and electrochemical properties. **R. Yamasaki***, H. Asakawa, T. Fukuma, T. Haruyama

1104. Synthesis and characterization of calix[4]arene micelles bearing four quaternary amines: Formation of regular polyhedral forms. **S. Yamada**, Y. Sanada, K. Sakurai*

1105. Mechanistic study on critical role of PEG crowdedness upon pDNA packaging into rod-shaped polyplex micelles. **K.M. Takeda***, K. Osada, T.A. Tockary, Q. Chen, A. Dirisala, K. Kataoka

1106. Structural and DNA interaction studies of a designed peptide-based vector. **J. Chauh***, K. Numata*

1107. Physicochemical characteristics and biocompatibility of self-assemble DNA-mimic brush polymers. **H. Kim***, J. Kim, M. Kim, J. Lee

1108. Development of carboxyl group modified b-1,3-glucans for protein delivery to antigen presenting cells. **D. Tanohata***, S. Mochizuki, N. Miyamoto, K. Sakurai

1109. Redox-responsive vesicles prepared from double armed alkyl ferrocene with aza-18-crown-6 ether molecules. **X. Wang***, N. Satio, B. Hatano, S. Murakami, T. Kijima

1110. Development of protein nanoparticles for sensitive biosensing. **Y. Ikeda***, Y. Mashimo, M. Mie, E. Kobatake

1111. Preparation of hollow nanocapsules for effective delivery of cationic sonosensitizers. **R. Teranishi**, E. Yuba, A. Harada, K. Kono*

1112. Development of temperature responsive hydrogel scaffold composed of self-assembling proteins for 3D cell culture. **Y. Mizuguchi***, Y. Mashimo, M. Mie, E. Kobatake

1113. Temperature responsibility and salt effect on sulfobetaine polymers and brushes. **Y. Mochizuki***, A. Sakamoto, H. Matsuoka

1114. Synthesis of entirely ionic diblock copolymers having betaine and formation behavior of PIC micelle. **T. Yagi**, K. Sasaoka, H. Matsuoka

1115. Characterizing micellar structures for hydrophilic dendron bearing calix[4]arene lipids. **G. Kubo**, S. Fujii, Y. Sanada, K. Sakurai*

1116. Development of pH-responsive polymeric micelles using amphiphilic block copolymer synthesized by mechano-chemical solid-state polymerization. **S. Kondo**, K. Tatematsu, Y. Sawama, Y. Sasai, Y. Yamauchi, M. Kuzuya

1117. Cationic copolymers to enhance deoxyribozyme activity for nucleic acid detection. **T. Oyanagi**, N. Shimada, A. Maruyama*

* Principle Author

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1118. Manipulating lipid bilayer membranes by peptide/cationic comb-type copolymer complex. **N. Kume**, T. Umegae, W. Sakamoto, N. Shimada, A. Maruyama*
1119. Disassembly and assembly of peptide fibrils via local mechanical perturbation. **A. Karsai***, T. Lanoue, F. Khouri, H. Malekan, W. Lin, V. Tran, D. Cox, X. Chen, G. Liu

1120. Ionic strength dependence of Calix [4] arene lipid. **S. Matsumoto**, S. Yamada, K. Sakurai*, Y. Sanada

1121. Interactions between DNA and cationic copolymers observed at single molecular level. **T. Takada**, A. Maruyama*, N. Shimada

1122. Examining the role of methionine oxidation on the soft-assembly of divalent peptide conjugate molecules and their use in the preparation of double and single helices of gold nanoparticles. **A. Merg, N. Rosi***

1123. Photoregulation of assembly and shape control of ionic gel particles. **S. Abe**, S. Tamesue, T. Mitsumata, N. Tsubokawa, T. Yamauchi*

1124. Enhancing enzyme stability by construction of polymer-enzyme conjugate micelles. N. Suthiwangcharoen, R. Nagarajan

1125. Design of self-assembling complexes based on formation-dependant physicochemical properties for application as biomaterials. **K. Hayashi***, H. Iwai, T. Shimanouchi, T. Kamei, H. Umakoshi, A. Kato, T. Iwasaki, H. Nakamura

1126. Self-assembly or quantum dots on biocompatible substance using dopamine polymerization. **F. Zhao***

1127. Binding of amphiphilic DNAs with different secondary structures to lipid bilayer membrane. **H. Yamaguchi**, K. Matsuzaki, T. Shibata, C. Dohno*, K. NAKATANI*

1128. Different mobility biofunctional nanosheet graphene oxides. **Y. Lai**, J. Tai, H. Wang, R. Ho, D. Tsai*

1129. Fabrication of chitosan-based polymeric nanocomplexes as a dual-functional drug carrier in combinational chemo-photodynamic therapy. **Y. Huang***

1130. Ligand-functionalized nanoparticles interactions in environmental health and safety. **Y. Lai**, C. Lai, J. Tai, T. Nguyen, .Wong, C. Lin, T. Tsai, H. Ho, P. Wang, Y. Liao, D. Tsai*

1131. Modulation of binding properties of DNA assemblies to lipid bilayer membrane. **C. Dohno***, S. Makishi, H. Yamaguchi, K. NAKATANI*

1132. Biomimetic in-situ study of the mineralization and demineralization of calcium carbonate with atomic force microscopy. **A. Reiber***

Thursday Afternoon

Hawaii Convention Center
313C

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: L. Bronstein, S. Sun

13:00 Welcoming remarks

13:05 – 1133. Nanoparticles, their hybrids and diodes for artificial photosynthesis, as heterogeneous organocatalysts, and for energy applications. **M. Antonietti***, D. Dontsova, J. Liu, M. Shalom

13:30 – 1134. Rational synthesis and assembly of nanocatalysts for energy application. **S. Sun***

13:55 – 1135. Green fabrication of gold and silver nanoparticles from lignin solution for high-value utilizations. G. Han, Z. Shen, X. Wang

14:10 – 1136. Magnetically recoverable catalysts based on magnetite nanoparticles: One phase or two?. N. Baird, K. Alibegovic, C. Braeger, N. Kuchkina, Z. Shifrina, C. Yuzik-Klimova, V. Matveeva, A. Sidorov, E. Sulman, L. Bronstein*

14:25 Intermission

14:40 – 1137. Effect of support on the activity of Ag-based catalysts for formaldehyde oxidation. **C. Zhang**

14:55 – 1138. Novel trimetallic nanocluster catalysts with a crown jewel structure for glucose oxidation. **N. Toshima***, H. Zhang, Y. Nozoe, Y. Shiraiishi

15:10 – 1139. Synthesis of zirconia in mesoporous silica and its catalytic property for methanol oxidative decomposition. **N. Shimoda**, K. Nakayama, S. Umebara, S. Satokawa*

15:25 – 1140. Precise synthesis of polyamine dendrimer-encapsulated Rh₅ carbonyl cluster for chemoselective reduction of aromatic nitro compounds. **Z. Maeno**, T. Mitsuodome, T. Mizugaki, K. Jitsukawa, K. Kaneda*

15:40 – 1141. Enantioselective C-H activation using ruthenium nanocatalysts: A DFT study. I. del Rosal, C. Taglang, B. Rousseau, G. Pieters, B. Chaudret, L. Maron, R. Poteau*

15:55 – 1142. Size-controlled, solvent-dispersible coordination polymer nanocrystals: Preparation and catalytic activity. **C. Meledandri**, K. Rodpurn, E. Tan, N.T. Lucas

16:10 – 1143. New insights on charge transfer in multi core nanoshell for photocatalysis. **A. Brito-Silva***, R.G. Sobral-Filho, Y. Wang, P. Wan, A.G. Brolo

16:25 – 1144. Novel synthesis of PtBi₂ alloy nanoparticles with exceptionally high electrocatalytic activity. **A.P. Angelopoulos***, P. Boolchand

16:40 – 1145. Hierarchical multicomponent catalysts: Structure design, function realization, and catalytic applications. **G. Wang***, H. Gao, D. Jia, J. Li, X. Zhang, L. Tan

Hawaii Convention Center
316A

Chemistry and Applications of Graphene (#39)

Organized by: Y. Chen, R. Haddon, K. Loh
Presiding: Y. Chen, H. Gao, R.C. Haddon

13:00 – 1146. Graphene, its heterostructures and beyond. **A. Geim***

13:30 – 1147. New carbon and related materials. **R.S. Ruoff***

13:50 – 1148. 2- and 3D carbon materials: From doped graphene to graphene oxide fabrics and more. **M. Terrones**

14:10 – 1149. Molecular-based proximity effects in graphene. **K. Takai***, T. Umebara, K. Nakamoto, A. Izumiyama

14:25 – 1150. Modulation of the Dirac point voltage of graphene by ion-gel dielectrics and its application to soft electronic devices. **y. shim**

14:40 – 1151. Multiscale modeling of gas molecules adsorption and penetration through multilayer graphene membrane. **G. Sergei***

14:55 Break

15:15 – 1152. 2D atomic crystals on transition metal surfaces: Silicene, germanene, and hafnene. **H. Gao**

15:35 – 1153. From graphene to phospherene: The 2D zoo. **A.H. Castro Neto***

15:55 – 1154. Structural diversity of bulky graphene materials. **X. Chen**

16:15 – 1155. Atomic and electronic properties of graphene-based heterostructure. **Y. Song**

16:30 – 1156. Development of graphene-based multifunctional hybrid structures: A Raman spectroscopy investigation. **E. Dervishi***, N.F. Hartmann, R. Silva, J. Yoo, Y. Lin, J. Sheehan, A. Chen, Q. Jia, H. Htoon, S.K. Doorn

16:45 – 1157. Wetting transparency of graphene in water. **A. Lazar**, D. Bratko, D. Vanzo, J.D. Driskill

Hawaii Convention Center
321A

Nanowires: Synthesis, Fundamental Properties and Novel Device Applications (#51)

Organized by: T. Yanagida, S. Hara, S. Jin, P. Yang, R. Agarwal, L. Lauhon, H. Zheng

Presiding: F. Ishikawa, T. Yanagida, P. Yang

13:00 – 1158. Nanowires, nanoplates, and nanofilms of 2D layered materials. **Y. Cui**

13:30 – 1159. Phase-equilibrium-dominated vapor-liquid-solid growth mechanism. **Q. Wu**, Y. Zhang, J. Cai, C. He, X. Wang, Z. Hu

14:00 – 1160. Theoretical guide on fabricating conducting/semitconducting molecular wires on semiconductor surface via in situ surface polymerization reaction. **J. Wang***, X. Yao, S. Yang

14:30 – 1161. Novel classical and quantum photonic devices by manipulating light-matter interactions in nanowires. **R. Agarwal***

15:00 Break

15:10 – 1162. Design strategy of metal oxide nanowires. **T. Kawai**

15:40 – 1163. Surface chemical approach to improving the air-stability of n-type semiconductor nanowires and nanotubes. **Y. Nonoguchi***, T. Kawai

16:10 – 1164. 1D metallic nanoparticles: Preparation, functionalization, and applications. **S.E. Hunyadi Murph**

16:20 – 1165. Electrochemical liquid-liquid-solid growth of semiconductor nanowires and microwires. **S. Maldonado***

16:30 – 1166. Hierarchically driven 1D metal oxide hybrid nanostructures as efficient electrocatalytic platforms toward electrochemical applications. **M. Kim***

16:40 – 1167. Metallic nanowires as new building blocks for flexible transparent electrodes synthesis, purification, and integration into functional devices. **J. SIMONATO***, C. Celle, A. Carella, C. Mayousse

16:50 – 1168. Gold ultrathin nanowires and nanorods: Synthesis, optical properties, and stability. **R. TAKAHATA**, S. Yamazoe, K. Koyasu, T. Tsukuda*

Hawaii Convention Center
318A

Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95)

Organized by: J. Kawamata, J. Choy, C. Detellier, H. Zhang, J. Huang, L. Wan
Presiding: J. Choy, M. Ogawa

13:00 – 1169. Function design via heteroassembly of inorganic nanosheets. **T. Sasaki***, Y. Ebina, M. Osada, R. Ma, T.C. Ozawa

13:30 – 1170. Bilayer silicate: Glassy defect structures and gas separation properties. **J. Schrier***

13:50 – 1171. Supramolecular thiophene nanosheets. **T. Ikeda***

14:10 – 1172. Environmentally benign synthesis of strongly coupled NiCo₂O₄-rGO hybrid nanosheets as a methanol-tolerant electrocatalyst for oxygen reduction reaction. **G. Zhang**

14:30 – 1173. Ultralight graphene-based architected elastomers. **D. Li**

14:55 Break

15:05 – 1174. Photoinduced electron transfer via metal oxide thin films fabricated by organic-inorganic hybrid Langmuir-Blodgett method. **H. Usami***

15:30 – 1175. Atomic manipulation of atomic oxygen of graphene epoxide. **T. Kim***

15:50 – 1176. Influence of graphene oxide supports on the stability and catalytic activity of metal nanoparticles. **S. Low**, V. Chen, Y. Shon*

16:10 – 1177. Synthesis, characterization, and intercalation properties of novel hybrid layered metal hydroxides modified with tris(hydroxymethyl)aminomethane. **Y. Kuroda***, T. Koichi, Y. Saito, A. Shimojima, H. Wada, K. Yamaguchi, N. Mizuno, K. Kuroda*

16:30 – 1178. Functional nanohybrid materials derived from phyllosilicates. **C. Detellier***, G. Kenne Dedzo

Hawaii Convention Center
321B

Applications of Ultrasound to Nanoscience (#150)

Organized by: K. Suslick, F. Grieser, M. Atobe, J. Yu, S. Jeong
Presiding: F. Grieser

13:00 – 1179. Size-controlled synthesis of polymer nanoparticles with tandem acoustic emulsification followed by soap-free emulsion polymerization. **M. Atobe**, K. Nakabayashi, M. Kojima, Y. Hirai

13:30 – 1180. Fluid-dynamical processes in the ultrasonic manipulation of milk fat globules. L. Johansson, T. Leong, P. Juliano, J. Jalal, J. Leontini, S. McArthur, R. Mawson, R. Manasseh*

14:00 – 1181. Ultrasonic assisted dissolution of switchgrass using active specific designed ionic liquid. **D. Grewell**, G.A. Kraus, M. Montalbo-Lombo

14:30 – 1182. Organic nanocrystals via sononchemistry: Host-guest chemistry, solid-state reactions, and pharmaceuticals. **L.R. MacGillivray**

15:00 – 1183. Room temperature sonochemical synthesis of red phosphorus/g-C₃N₄ hybrid nanosheets for photocatalytic hydrogen evolution. **J. Yu***

15:30 – 1184. Separation of nanoparticles from suspensions with ultrasonic atomization. **S. Ni***

16:00 – 1185. Design, synthesis of nanoparticles and fabrication of polymer nanocomposites. **V.K. Rangari***, S. Jeelani

16:30 – 1186. Ultrasonic spray synthesis of functional, shape-controlled nanomaterials. **S.E. Skrabalak**

Hawaii Convention Center
322AB

Current and Future Applications of Nanotechnology in the Oil Industry (#197)

Organized by: W. Wang, K. Lee, J. Ordóñez-Varela, M. Kanj, T. Jiang
Presiding: M.E. Poitzsch

13:00 – 1187. Understanding electronic properties of coherent 2D nanostructures with multi-pbe STM spectroscopy. **A. Li**

13:30 – 1188. Highly shear thinning nanoparticle solutions in water. **J. Weston**, B. Grady, J. Harwell, D. Resasco

13:55 Break

14:10 – 1189. Synthesis and applications of near-infrared persistent luminescent nanoparticles. **Z. Pan***, F. Liu, Y. Chuang, Y. Liang, Y. Chen

14:40 – 1190. New strategy for designing silver(I) coordination complexes for olefin/paraffin separations. **M.G. Cowan**, W. McDowell, H.H. Funke, Y. Kohno, D. Gin, R.D. Noble

* Principle Author

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TECHNICAL PROGRAM

15:05 – 1191. Progress and challenge on detection of nano-agents in reservoir characterization. **W. Wang***

15:30 closing remark

Hawaii Convention Center
319A

Self-organization of Membrane Systems (#259)

Organized by: D. Sasaki, K. Morigaki, I. Kooper
Presiding: I. Kooper, M. Lösche

13:00 – 1192. Nanolipoprotein particles entrapped within nanoporous silica gel. **W. Zeno, S.H. Risbud, M.L. Longo**

13:30 – 1193. Lipid membrane reorganization induced by self-assembly of a toxin. **N. Yilmaz**

13:50 – 1194. Supported lipid bilayer chromatography and sensing platforms. **P. Cremer**

14:20 – 1195. Submicron domains in phosphatidylinositol-containing supported lipid bilayers and their roles in protein assembly. T. Motegi, K. Takiguchi, Y. Tanaka-Takiguchi, **R. Tero***

14:40 – 1196. Improved models of the gram negative bacterial outer membrane. **S.A. Holt*, A. Le Brun, L. Clifton, J.H. Lakey**

15:10 break

15:15 – 1197. Sparsely tethered lipid bilayer membranes as a model for biomembrane function. **B.A. Cornell***

15:45 – 1198. Polymer-tethered single- and multilipid bilayers as model membranes and biomimetic-mimicking cell substrates of adjustable dynamic and mechanical properties. **C.A. Naumann*, C. Lin, Y. Ge, L. Lautscham, W.H. Goldmann, B. Fabry**

16:05 – 1199. Effects of oxidative stress on model cellular membrane and protein interactions. **D.J. McGillivray*, J.J. Knobloch, Y. Xun, A.R. Nelson, N. Kirby**

16:35 – 1200. Tethered bilayer lipid membranes as a platform for functional membrane protein insertion. J. Zieleniecki, Y. Nagarajan, J. Rongala, S. Waters, M. Hrmova, **I. Kooper***

16:55 Concluding Remarks

Hawaii Convention Center
318B

Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308)

Organized by: R. Morandotti, D. Moss, F. Omenetto, N. Tsutsumi, K. Alamgir, K. Char, A. Facchetti
Presiding: K. Char

13:00 – 1201. Development of high performance printed polymer integrated circuits. **Y. Noh**

13:30 – 1202. Emission features of organic oligomer crystals equipped with 1D diffraction gratings. **T. Yamao***

14:40 – 1203. Fabrication of polymer-based arrayed waveguide gratings for upconversion transparent displays.

S. Watanabe, T. Asanuma, H. Hyodo, K. Soga, M. Matsumoto, S. Takafumi

14:20 – 1204. Synthesis of new acrylamide-based block copolymers and their application to nanolithography. **Y. Han***

14:40 – 1205. Optochemical organization: Using light to transfer and encode information in a photopolymer.

K. Saravananuttu*, A. Hudson, M. Ponte

15:00 Break

15:10 – 1206. Bulk heterojunction perovskite hybrid solar cells. **X. Gong**

15:40 – 1207. Morphology control of organic-inorganic perovskite layers by hot isostatic pressing for efficient planar solar cells. **T. Matsushima***, T. Fujihara, C. Qin, Y. Esaki, S. Hwang, S. D. Sandanayaka, C. Adachi

16:00 – 1208. Sn perovskite photoconversion devices with infrared sensitivity. **S. Hayase***

16:20 – 1209. Influence of processing and post-processing conditions on charge generation and recombination of thin-film lead-halide perovskites for electrooptical applications. **S.A. Bretschneider, I. Hermes, S. Weber, F. Laqua***

16:40 – 1210. Real-space observation of charge distribution in perovskite solar cells. **V.W. Bergmann*, S.A. Weber, F.J. Ramos, M.K. Nazeeruddin, M. Grätzel, S. Ahmad, R. Berger**

Hawaii Convention Center
319B

Membranes and Nanotechnologies for Energy and Environment Applications (#317)

Organized by: H. Park, B. Freeman, B. McCloskey, J. McGrath, A. Hill, A. Higuchi, Y. Lee

13:00 – 1211. Dramatic nanofluidic properties of carbon nanotube membranes for environmental and energy applications. **B.J. Hinds***

13:30 – 1212. Gas permeation through 1 nm thick carbon nanomembranes. A. Beyer, V. Chinarray, X. Zhang, S. Shishatskiy, J. Wind, V. Abetz, **A. Goelzhaeuser***

13:50 – 1213. Ultrathin gas selective membranes based on metal-organic framework nanosheets for H_2/CO_2 separation. Y. Peng, Y. Li, **W. Yang**

14:10 – 1214. Speed limits of gas/vapor/liquid: Has graphene laid the ultimate transport pathways?. **A. Thornton*, A.J. Hill, H. Park, M. Majumder**

14:30 – 1215. Biomimetic selective ion transport through graphene oxide membranes functionalized with ion recognizing peptides. S. Kim, J. Nham, Y. Jeong, C. Lee, S. Ha, H. Park, **Y. Lee***

14:50 – 1216. Mass transport under graphitic nanoconfinement, continuous or discontinuous. **H. Park***, S. Youn, J. Buchheim, R.M. Wyss, A. Droudian, M. Lokes

15:20 – 1217. Carbon molecular sieve gas separation membranes derived from novel nanostructured immiscible polymer blends. N.P. Panapitya, C.J. Gilpin, I.H. Musselman, K. Balkus, **J.P. Ferraris***

15:40 – 1218. Multilayer polymer nanocomposite thin films capable of size selective gas separation. **J. Grunlan***, B. Wilhite

16:00 – 1219. Multiscale architected polymeric membranes with tunable separation properties. **P.J. Yoo***

16:20 – 1220. Plasticization-tolerant graphene oxide membranes for CO_2 separations. **H. Kim**, H. Yoon, J. Park, B. Freeman, H. Park

16:40 – 1221. Architecting porosity for efficient molecular transport in membranes. **A.J. Hill, A. Thornton**

Hawaii Convention Center
316C

Ceramic Materials and Processing for Advanced Applications (#341)

Organized by: F. Rosei, A. Vomiero, Y. Tachibana, C. Raston, H. Zhang

13:00 – 1222. Plasmonic nanoparticles to boost the response dynamic and sensitivity of optical gas sensors based on metal oxide. **A. Martucci**

13:30 – 1223. Flexible chemical processing: Multiple WO_3 typologies from a single precursor and their gas-sensing properties. **M. Epifani***, E. Comini, R. Diaz, T. Andreu, J. Arbiol, P. Siciliano, G. Faglia, J.R. Morante

14:00 – 1224. Catalytic activity of perovskite-type oxide synthesized by assisting exothermic ligand oxidation of heteronuclear cyano complex. **H. Wada**, D. Sánchez-Rodríguez, S. Yamaguchi, H. Yahiro

14:15 – 1225. Preparation of zinc oxide particles in the presence of anionic surfactants. **Y. Iizuka***, H. Shibata, T. Ogura, A. Fujimori, K. Hashimoto

14:30 – 1226. Comparison of oxygen sorption/desorption behavior between $\text{Sr}-\text{FeO}_{3-\delta}$ and $\text{BaFeO}_{3-\delta}$. **H. Ikeda, A. TSUCHIDA, N. MIURA***

14:45 coffee break

15:00 – 1227. Solution routes to complex oxide, metal, and composite nanomaterials. **G. Westin***

15:30 – 1228. Ceramics for metal-organic frameworks based devices. **P. Falcaro**

16:00 – 1229. Hybrid carbon and other 2D materials by Pulsed Laser Deposition with applications in electron emitters and PEM fuel cells. **D.H. Chua**

16:30 – 1230. Sol-gel synthesis of rhodium substituted ϵ -iron oxide nanoparticle exhibiting zero-field ferromagnetic resonance. **A. Namai, M. Yoshiyuki, S. Ohkoshi**

16:45 – 1231. Is hysteresis truly a problem for perovskite solar cells?. **A.K. Jena***, A. Kularki, A. Kogo, Y. Numata, M. Ikegami, T. Miyasaka

Hawaii Convention Center
316B

Materials for the Mitigation of Chemical Hazards (#388)

Organized by: J. DeCoste, G. Peterson, J. Becker, M. Biggs, L. Croll, K. Walton
Presiding: G. Peterson

13:00 – 1232. Highly adsorptive, MOF-functionalized fiber mats for hazardous gas capture enabled by atomic layer deposition. **G. Parsons***, J. Zhao, W. Nunn, P. Lemaire, D. Lee, C. Oldham, H. Walls, G. Peterson

13:30 – 1233. *In operando* studies of CuO_x and MoO_x model surfaces for application as chemical warfare agent destruction catalysts. **L. Trochaud**, A. Head, Y. Yu, O. Karşıloğlu, M. Hartl, B. Eichhorn, H. Bluhm

13:50 – 1234. Removal of sulfur mustard gas surrogate under visible light on the surface of hydrous ferric oxide/graphite oxide composites. **J. Arcibar Orozco***, T.J. Bandosz

14:10 – 1235. Microwave-assisted synthesis, characterization, and photocatalytic properties of highly dispersed SiO_2/ZnO core-shell nanocomposite particles. **N.M. Bahadur***, F. Kurayama, T. Furusawa, M. Sato, N. Suzuki

14:30 – 1236. Adsorbent-nanofibre composite materials: Concepts for broad spectrum chemical protection. **D. Nielsen***, M. Jamriski, R. Hebdon, E. Micich, J. Freeman

15:00 Break

15:10 – 1237. CWA surrogates decontamination on metal (hydro)oxide/graphite oxide adsorbents: Engaging chemical reactivity, porosity, conductivity, and visible light activity. **T.J. Bandosz***, J. Arcibar Orozco, D. Giannakoudakis

15:40 – 1238. Sol-gel synthesis of robust hierarchical porous monolithic metal(IV) phosphate materials for efficient ion adsorption. **Y. Zhu**, K. Yoneda, T. Shimizu, K. Kanamori*, K. Nakanishi*

16:00 – 1239. Electrospin composite nanofibers for enhanced photocatalytic degradation of environmental toxins. **D.L. McCarthy**, J. Liu, J. Tolin, J. Troiano, J. DeCoste, W.E. Bernier, **W.E. Jones***

Hawaii Convention Center
314

Design of Innovative Photochromic Applications (#399)

Organized by: J. Abe, T. Kawai, Y. Yokoyama, N. Branda, F. Raymo, W. Zhu
Presiding: F.M. Raymo

13:00 – 1240. Photo-motion and photo-polism in photochromic systems. **D. Bassani**

13:20 – 1241. Tailor-made photochromic molecules/proteins for super-resolution microscopy. **J. Hoffens***, p. dedecker, B. Moeyaert, S. Duwé

13:40 – 1242. Amplified photoswitching in fluorescent photochromic molecules and nanomaterials. **K. NAKATANI***, R. METTIER, S. MAISONNEUVE, J. XIE, P. Yu, K. OUEHNA-OUADAH, J. SU, T. Fukaminato, J. PLACIAL,

A. BROSSEAU, J. AUDIBERT, R. PANUS

14:00 – 1243. Reversible force visualization on luminescent elastomer films. **S. Saito***, S. Nobuse, S. Yamaguchi, H. Yabu*, Y. Saito

14:20 – 1244. Development of photochromic molecules. **T. Fukaminato***, T. Hirose, K. Matsuda, M. Irie

14:40 Break

14:55 – 1245. Photochemical strategies to activate fluorescence. **F.M. Raymo**

15:15 – 1246. Switchable fluorescent probes for sensing and imaging biomolecules. **T. Yi, G. Lv, K. Liu**

15:35 – 1247. Photoresponsive molecules and materials for controlling chemistry and biochemistry. **N. Branda***, T. Wu, D. Wilson

15:55 – 1248. Synergetic effects in photochromic nanoparticles. P. Girard, K.E. Snell, T. Gallavardin, L. Lartigue, J. Duval, F. Lagugné-Labarthet, E. Ishow

16:15 – 1249. Photomechanical actuators of photochromic diarylethene crystals. **S. Kobatake**, D. Kitagawa

Hawaii Convention Center
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Advances in Organic Light-Emitting Diodes (#409)

Organized by: J. Bredas, C. Adachi, K. Wong, V. Yam, P. Burn, J. Kim
Presiding: E.R. Bittner

13:30 – 1250. Theory of exciton radiative and non-radiative decay for OLEDs materials. **Z. Shuai***

14:40 – 1251. Accelerated discovery of OLED materials through atomic-scale simulation. **M.D. Halls***, D.J. Giesen, T.F. Hughes, A. Goldberg, Y. Cao, H.S. Kwak, G.P. Dathar, J.L. Gardarin, S.R. Kimura, D. Yoshidome

14:20 – 1252. Computational design of host and guest molecules for OLED active layers. **P. Winge***, M. Hong, H. Sun, J. Bredas

14:40 – 1253. Excitonics of phosphorescent, fluorescent, and TADF-based OLEDs: A Monte Carlo simulation approach.

H. van Eersel, M. Mesta, M. Carvelli, P. Bobbert, R. Janssen, R. Coehoorn

15:00 – 1254. Hyper-phosphorescence: Boosting the limits of blue phosphorescent technology. **C. Lenhardt**, F. May, M. Zhang, G. Wagenblast, H. Mangold, G. Battagliarin, T. Holcombe, I. Münster

15:30 Break

15:40 – 1255. New materials: Synthesis, photophysics, and high efficiency organic light-emitting devices. **M.R. Bryce***

16:10 – 1256. Making use of triplet excitons in organic electronics: Thermally activated delayed fluorescence and bioluminescence. **S. Reineke***

16:40 – 1257. Fluorescence-based organic light-emitting diodes with high efficiency and reliability. **H. Nakanotani**, C. Adachi

* Principle Author

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17:00 – 1258. Development of high performance OLEDs for general lighting.
J. Kido*

Hawaii Convention Center
317B

The Frontiers of Geometrically Frustrated Magnetic Materials (#430)

Organized by: C. Wiebe, C. Ling,
J. Gardner, H. Zhou

13:00 – 1259. Giant magnetoelasticity at a spin gap transition in the 5d oxide Ba₃Bil₂O₉.
C.D. Ling*

13:40 – 1260. Dugganites: An experimental realization of a molecular 2D triangular Heisenberg antiferromagnet?
H. Silverstein*, A. Sharma, h. zhou,
C. Wiebe

13:55 – 1261. High field ESR study of Kagome lattice antiferromagnet Cr-jarosite single crystal. **H. Ohta***,
S. Okubo, R. Nakata, S. Ikeda,
N. Takahashi, T. Shimokawa, T. Sakurai,
W. Zhang, K. Okuta, S. Hara, H. Sato

14:10 – 1262. Study of new beryllium substituted langasites A₃Ga₃Ge₂BeO₁₄ (A=Pr,
Nd, Sm).
A. Sharma*, C. Wiebe

14:25 – 1263. Synthesis and properties of new mixed-anion geometrically frustrated magnets.
J.P. Attfield, L. Clark

15:10 Coffee Break

15:25 – 1264. Doppelgängers amongst the double perovskites. **J. Greedan***,
C. Thompson, C. Marjesson, B. Gaulin,
G. Luke, G. Nilson, C. Wiebe

16:05 – 1265. Understanding the interplay between the magnetic and crystal structure in Sr₂YRuO₆.
B.J. Kennedy*,
P. Kayser, B. Ranjbar, M. Avdeev

Hawaii Convention Center
320 Theatre

Self-assembled Biofunctional Nanomaterials (#433)

Organized by: R. Nagarajan, K. Sakurai,
H. Chen

13:00 – 1266. Protein-polymer co-assembled nanoparticles for catalysis and vaccine applications.
Q. Wang*

13:30 – 1267. Control over charge and charge density in micelles from ABC tri-block terpolymers: Effects on interaction with cells.
F.H. Schacher*

14:00 – 1268. Sugar and spice: Natural bio-functional materials from self-assembling polysaccharides.
B. Williams*

14:30 – 1269. Enzyme-responsive micellar nanoparticles.
N. Giannesci

15:00 Break

15:10 – 1270. Amphiphilic polycaprolactones for micellar delivery of anticancer drugs.
m.C. Stefan*

15:30 – 1271. Innate immunity peptides and self-assembly.
g. wong*

16:00 – 1272. Simple approach to synthesize multifunctional hybrid nanocomposites for biomedical applications.
Y. Li*,
D. Niu, Y. Gao, X. Zhang

16:20 – 1273. Manipulation of immune responses by the hydrophobicity of nanomaterial composed of amphiphilic poly(-glutamic acid).
F. Shima*, T. Akagi,
M. Akashi

16:40 – 1274. Lipid self-assembly nanoparticles as theranostic drug delivery and medical imaging agents.
C.J. Drummond*, X. Mulet, C.E. Conn,
C. Fong, M. Moghaddam, N. Tse,
D. Kennedy, R.A. Caruso, S. Sagnella,
X. Gong, J. zhai

Hawaii Convention Center
317A

Application of Luminescent Materials for Radiation Detection (#442)

Organized by: K. Asai, J. Zhang,
T. Yanagida, S. Kasap
Presiding: K. Asai

13:00 – 1275. Development of fast scintillators exhibiting auger-free luminescence.
M. Koshimizu

13:40 – 1276. Radiation resistance and improved response times of bulk ZnO single crystals after gamma-ray irradiation.
K. Yamanoi

14:00 – 1277. Surface vs. bulk self trapped exciton (STE) in the radioluminescence of calcium fluoride nanoparticle.
R. Sammynaike*

14:40 – 1278. Analysis of thermoluminescence data and future uses.
K. SHINSHO

15:20 – 1279. Radiophotoluminescence from Sm-doped glasses and glass-ceramics for large-dose, high-resolution radiation dose measurement in microbeam radiation therapy.
G. Okada, A. Edgar,
J. Ueda, S. Tanabe, C. Koughia,
F. Chicilo , D. Tonchev, G. Belev,
T. Wysokinski, D. Chapman, S. Kasap*

16:00 – 1280. Lithium-containing amorphous materials for radiation detection.
H. Masai*, T. Yanagida

16:40 – 1281. Luminescence properties of new layered mixed-anion compounds Ba₃RE₂O₅.
M. Tatsuda, H. Ogino,
T. Yanagida, Y. Fujimoto, J. Shirayama,
K. Kishio

Thursday Evening

Hawaii Convention Center
318B

Nanocrystal Synthesis, Characterization, Assembly and Applications (#34)

Organized by: R. Tilley, S. Skrabalak,
T. Hyeon, T. Nann, T. Adshri

19:00 – 1282. Shape directed synthesis of Pt and Pd nanoparticles.
R.M. Richards,
G. Leong, A. Ebonsiar, M. Schulze,
M. Strand, D. Maloney, S. Frisco, C. Ngo,
H. Dinh, B. Pivovar, G. Gilmer,
S. Kodambaka, C. Ciobanu

19:15 – 1283. Studying perovskite-based solar cells with high resolution in-situ microscopy.
J.A. Aguilar, S. Wozyk,
W. Zhou, K. Zhu, T. Holesinger, T. Aoki,
M. Al-Jassim

19:30 – 1284. Low-temperature synthesis of compositionally complex scheelite-structured nanocrystals.
S.P. Culver*,
R. Brutcher

19:45 – 1285. Optimizing the seed mediated growth of gold nanorods.
B.D. Gates*,
I.W. Guo

20:00 – 1286. Characterizing the effects of dithiocarbamate ligands on CdSe nanocrystals.
A.M. Munro*

20:15 – 1287. Alloy nanocatalysts.
J. Zeng

20:30 – 1288. Efficient selective catalysis via supported Pt-based nanocatalyst with specific crystal facets.
K. Tang*, J. Zhu,
W. Yang, Y. Ye

Hawaii Convention Center
Halls I, II, III

Nanowires: Synthesis, Fundamental Properties and Novel Device Applications (#51)

Organized by: T. Yanagida, S. Hara,
S. Jin, P. Yang, R. Agarwal, L. Lauhon,
H. Zheng

Presiding: N. Fukata, S. Hara,
F. Ishikawa, T. Yanagida

Poster Session

19:00 – 21:00

1289. Metallic glass nanowires: Formation, fundamental properties, and applications.
K. Nakayama*

1290. Electrodeposition of crystalline Si nanowires at low temperatures.
L. Ma,
S. Lee, S. Maldonado*

1291. Fabrication of flexible transparent conductive electrode using curved copper nanowires.
Z. Yin, S. Cho, D. You,
Y. Ahn, Y. Yang, J. Yoo, Y. Kim*

1292. Hybrid SiNW-based solar cells and hydrogenation for efficiency enhancement.
W. Jevasuwan, K. Nakajima,
Y. Sugimoto, N. Fukata

1293. Fabrication of fine sodium titanate nanowires with high Si ion exchange properties.
N. Asao*, Y. Ishikawa,
S. Tsukimoto, K. Nakayama

1294. Study of influential factors in polyol synthesis of silver nanowires assisted by single-mode microwave irradiation.
S. Saito*, M. Sato, T. Furusawa,
N. Suzuki

1295. Fabrication of Pd-Ni alloy nanorings using a molecular assembly soft-template of a long-chain amidoamine derivative.
A. Shoji

1296. Fabrication and catalytic activity of Pd-Cu nanowires with network structure.
H. Ikeda

1297. Enhanced neuronal growth by intracellular stimulation.
J. Na, J. Kwon,
M. Hong, I. Kim, H. Choi*

1298. Gigantic reduction of energy consumption of volatile molecule sensors by pulse-heating of Sn₂O₅ nanowire device with picosecond thermal relaxation time.
G. Meng, K. Nagashima, F. Zhuge,
M. Kanai, Y. He, T. Takahashi, K. Uchida,
T. Yanagida

1299. Aligned synthesis of the geometrically-controlled carbon microcoil.
G. Kang*,
J. Lee, S. Kim

1300. Band gap engineering of III-V nanowires and nanobelts.
X. Zhang, L. Ma,
H. Tan, P. Ren, A. Pan

1301. Double-helical Au nanowires synthesized using a hydrogel template composed of two organogelators.
M. Nakagawa*, T. Kawai

1302. Modulated transport properties in B-doped Si nanowires via rationally designed dopant inhomogeneity and its application in piezoelectrics.
F. Zhuge,
N. Fukata, K. Uchida, K. Nagashima,
M. Kanai, G. Meng, Y. He, S. RAHONG,
X. Li, T. Kawai, T. Yanagida

1303. Photonic sintering of copper nanowires for flexible transparent conducting electrodes.
K. Woo*, Z. Zhong, Y. Choi,
S. Kwon, Y. Jang, I. Kim, J. Moon

1304. Preparation of metal nanostructures for ultrafast electrochromic response.
Y. Tanaka

1305. Preparation and electrical properties of molybdenum blue bronze nanoribbons.
T. Nishida*, T. Okazaki, K. Eda,
T. Yanagida

1306. Optical characteristics and electromagnetic simulations of metal nanostructures. **S. Akimoto**

1307. Unveiled experimental design rule for vapor-liquid-solid oxide nanowire growth.
A. Klamchuen, K. Nagashima*,
M. Suzuki, H. Yoshida, M. Kanai,
G. Meng, F. Zhuge, Y. He, S. Kai,
S. Takeda, T. Kawai, T. Yanagida

1308. Nanowire alignment on micrometer scale hydrophilic patterns by blade-coating method.
Y. He, K. Nagashima,
M. Kanai, G. Meng, F. Zhuge,
S. RAHONG, X. Li, T. Kawai, T. Yanagida

Hawaii Convention Center
321A

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

Organized by: M. Nyman, Y. Li, T. Ozeki,
C. Ritchie
Presiding: P.I. Molina

19:00 – 1309. Polyoxometalate paneling from (Mo₂O₅S₂) coordination.
E. Cadot*,
S. Floquet

19:20 – 1310. Chemistry inside the capsule: Ligand exchange for (W₇Mo₆) keplerate.
V.S. Korenev*, M.K. Soboleva

19:40 – 1311. Electrical conduction of polyoxometalate-based solid: Non-covalent wiring of clusters to networks.
R. Tsunashima

20:00 – 1312. Polyoxometalate complexes of anatase-TiO₂ cores in water.
M. Raula,
G. Gan Or, Y. Wang, I. Weinstock*

20:20 – 1313. Visible-light-responsive photoredox catalysis of silicogitostates.
K. Suzuki, J. Jeong, F. Tang,
Y. Kikukawa, K. Yamaguchi, N. Mizuno

20:40 – 1314. Construction of polyoxometalate-based porous materials for heterogeneous catalysis.
Y. Wang, H. Zang,
H. Tan, Y. Li*

Hawaii Convention Center
Halls I, II, III

Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95)

Organized by: J. Kawamata, J. Choy,
C. Detellier, H. Zhang, J. Huang, L. Wan
Presiding: J. Kawamata, Y. Suzuki

Poster Session

19:00 – 21:00

1315. Plasmon resonances in 2D MoS₂.
K. Kalantar-zadeh*, J.Z. Ou, Y. Wang,
T. Daeneke

1316. Unraveling orientation distribution and merging behavior of monolayer MoS₂ domains on sapphire.
Q. Ji*, Y. Zhang*,
z. Liu*

1317. Stability of water-based MoS₂ nanosheets dispersion.
E. Mieda,
M. Horikawa, S. Shimada, R. AZUMI,
A. Ando*

1318. Investigation of two-solvent grinding assisted liquid phase exfoliation of layered MoS₂.
E.P. Nguyen*,
K. Kalantar-zadeh, T. Daeneke,
B.J. Carey, S. Zhuiykov

1319. Two solvent grinding sonication method for the synthesis of 2D tungsten disulfide flakes.
B.J. Carey*

1320. Growth and optical properties of high-quality monolayer WS₂ on graphite.
Y. Kobayashi, S. Sasaki, S. Mori,
H. Hibino, Z. Liu, K. Watanabe,
T. Taniguchi, K. Suenaga, Y. Maniwa,
Y. Miyata*

1321. Molybdenum disulfide based nanocomposite material synthesis, characterization, and sensing applications.
R. Clark, T. Daeneke, K. Kalantar-zadeh*

1322. Synthesis of graphene flake and nitrogen-doped graphene-like nanoflakes by pyrolysis of polyacrylonitrile.
H. Kwon*,
S.O. Cho

1323. CVD growth of large single crystal graphene.
L. Lin, H. Peng, z. Liu

1324. Raman spectroscopy of graphene grown on various metals.
Y. Nakata,
J. Takahashi, H. Kato, Y. Homma

1325. Origin of high efficient graphene heater induced by electromagnetic wave.
S. Kang*, H. Choi, S. Park, B. Hong*

1326. In plane step-edge growth of graphene in a STEM.
Z. Liu*, Y. Lin, P. Chiu,
S. Iijima, K. Suenaga

1327. Remarkable improvement of the electrode performance of Mn₃O₄-graphene nanocomposites upon the incorporation of exfoliated inorganic nanosheets.
K. Adpakpong*, S. Hwang

1328. Preparation and characterizations of graphene-clay composite film.
T. Nakamura*, H. Nanjo, T. Ebina, R. Ishii

1329. Large-area single layer exfoliation of graphene oxide via Couette-Taylor flow reactor.
W. Park*, H. Kim*, S. Yoo,
S. Kim, Y. Do, D. Yoon, **W. Yang***

1330. Synthesis of metal nanoparticle/graphene nanocomposites using atmospheric-pressure-microplasma-assisted electrochemistry.
H. Huang*, **J. Yang**,
W. Chiang

* Principle Author

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onlineprogram

- 1331.** Introduction of 1-aminopyrene to graphene oxide via covalent bonding.
M. Morimoto, Y. Matsuo*
- 1332.** Revealing coordination chemistry of metallic molecules with N-doped graphene: Implications for oxygen reduction reaction reactivity of organometallic metal- $\text{O}_4^{\text{-}}\text{N}^{\text{-}}$ -species. Y. Shim, s. Lee, s. kim, J. Oh, S. Park
- 1333.** Opportunities for sp^2 hybridized carbon nitride. P. Persson, J. Palisaitis, A. Kakanakova-Georgieva
- 1334.** Water-dispersible, atomically thin carbon nitride-based nanodots and their performances as bioimaging probes. J. Oh, s. Park, Y. Shim, D. Kim, S. Park
- 1335.** Development of the novel film actuator with carbon nitride polymers. H. Arazoe, D. Miyajima, T. Aida
- 1336.** Controlled growth of planar boron nitride on tailored thin film substrates using pulsed laser deposition. J. Terry, D. Velazquez, R.L. Seibert
- 1337.** Radiosotope Co-57 introduced layered double hydroxide as radioisotopic cell labeling nanoparticles. T. Kim, J. Lee, S. Paek, J. Park, J. OH*
- 1338.** Size and surface charge dependent flocculation of layered double hydroxide nanomaterials with *Microcystis aeruginosa*. T. Kim, I. Hong, J. OH*
- 1339.** Direct preparation and stacking of 2D Mg-Al-LDHs crystals. D. Liang*, X. Yang
- 1340.** Injectible 2D nanovehicle for chemotherapy. G. Choi, J. Choy*
- 1341.** SERS active gold nanostructure by synchrotron radiation induced photochemical reaction. T. Matsumoto, I. Okada, I. Sakurai, Y. Utsumi, A. Yamaguchi
- 1342.** Synthesis of metal nanoparticles within interlayer space of titania nanosheet film. K. Sasaki, S. Kawamura, K. Saito, M. Yagi, R. Sasai, T. Yui
- 1343.** Magnetic properties of antidot films in function of size. R. Levin*, A. Ibarra, S. Vojkovic, J.C. Denardin
- 1344.** Structural evolution of $\text{Cu}(\text{OH})_2$ micro-crystals formed on copper surface. K. Matsui*, A. Mochida
- 1345.** Anisotropic hydrogel with electrostatic repulsion between cofacially aligned nanosheets. M. Liu*
- 1346.** Homogeneous incorporation of inorganic nanoparticle into hydrogel through in situ electrophoretic precipitation. G. Gwak, N. Kwon, W. Lee, S. Paek, S. Kim, J. OH*
- 1347.** Crystal growth of a layered silicate on amorphous silica fibers. K. Shimizu, T. Okada
- 1348.** Quasi planar hexacoordinate carbon in Be_2C monolayer: A global minimum structure. Y. Li*
- 1349.** Epitaxial growth of methyl-terminated germanene multilayers on silicon. Y. Yasutake*, S. Fukatsu
- 1350.** In situ crystallization of an Al-containing layered silicate on monodisperse spherical colloidal silica particles. M. Sueyoshi, T. Okada
- 1351.** Toward in situ observation of the formation process of mesoporous films with surfactant molecules by using confocal laser scanning microscope. T. Kimura*, M. Shintate, N. Miyamoto
- 1352.** Mechanochemical lithiation of layered polysilane. M. Ohashi, H. Nakano
- 1353.** Content and functional regulation of nitrogen ligands within 2D covalent organic frameworks for controllable mono-metallic or bimetallic docking. Y. Gao*, W. Leng, Y. Peng
- 1354.** Adsorption-desorption behavior of In^{3+} on clay-poly(*N*-Isopropylacrylamide) nanocomposite. Y. YASHIRO
- 1355.** Studies of lanthanide bearing on titanate nanosheets: Niobium addition effects on the bearing reaction and the fluorescence. D. Yoshioka*, Y. Nishimura, K. Katsurata
- 1356.** Synthesis of silver nanoparticle within interlayer space of layered semiconductor. S. Kawamura, K. Sasaki, F. Takagi, K. Saito, M. Yagi, W. Norimatsu, R. Sasai, T. Yui
- 1357.** Preparation of Rh-doped titanate nanosheet/porphyrin hybrid thin solid film and its photochemical characterization. W. Soontornchaiyakul*, R. Sasaki, H. Usami
- 1358.** Largely enhanced activity of Au/TiO₂ plasmonic photocatalyst and h-BN nanosheet mixture. Y. Ide*, K. Nagao, K. Komaguchi, Y. Sugahara, Y. Bando, D. Golberg
- 1359.** Fabrication and photocatalysis of organosilica-titanium oxide hybrid particles. Y. Makii, Y. Ide, T. Okada
- 1360.** Remarkably enhanced photocatalytic activity of layered titanate by simple mixing with commercial TiO₂ particles. K. Saito, M. Kozeni, Y. Ide*, M. Ogawa, Y. Sugahara*
- 1361.** Dielectric properties of molecularly-thin titania nanosheets. D. Ogawa, Y. Kim, K. Atsukata, M. Osada*, T. Fukumura, T. Hasegawa*, T. Sasaki*
- 1362.** Preparation of single structured ionic cyclotetrasiloxanes forming 2D layered aggregates. Y. Kaneko*, S. Kinoshita, S. Watase, K. Matsukawa
- 1363.** Functionalization of thin montmorillonite films with cyclodextrin/dye supramolecular complexes. M. Matejčík*, A. Čížmová, M. Janek, J. Kawamata
- 1364.** Nanosheets-based entities self-assembled from double calixarene and amines. A. Hitoshi, T. Nagatsuka, R. Jin
- 1365.** Precise control of the stacking pitches of alternate layered nanostructure composed of various metal oxide nanosheets. T. Ano*, F. Kishimoto, D. Mochizuki, M. Maitani, E. Suzuki, Y. Wada
- 1366.** Controllability of photoinduced charge separation at alternate layered nanostructure synthesized with thiol-ene click reaction of two metal oxides nanosheets. F. Kishimoto*, T. Ano, D. Mochizuki, M. Maitani, E. Suzuki, Y. Wada
- 1367.** Tuning the electronic and optical properties of phosphorene via molecular doping: A first principle calculation. Y. Jing*
- 1368.** Organoclays in water cause interlayer expansion that facilitates caffeine adsorption. T. Okada*
- 1369.** Synthesis of a nanosheet comprising a 4-way porphyrin-dipyrromethane hybrid ligand and zinc ions. T. Yagi*, R. Sakamoto, H. Nishihara
- 1370.** Investigation on mechanism of self-fluorescence quenching reaction on the clay surface. N. Morita, Y. Ohtani, T. Shimada, S. Takagi
- 1371.** Environment responsive fluorescence quenching behavior of clay nanosheet-organic dye composite. R. Honma, T. Fujimura, T. Shimada, S. Takagi
- 1372.** Development of chiral hybrid thin film composed of magnesium porphyrin and inorganic layered material. T. Fujimura*, T. Shimada, R. Sasai, S. Takagi*
- 1373.** Flexible and transparent free-standing metal nanosheets fabricated by UV irradiation onto Langmuir monolayers of nanoparticles. T. Nishimura*, T. Kawai
- 1374.** Optical, mechanical, and electronic properties of a 2D silver nanoparticle sheet. P. Wang, S. Araki, S. Ryuzaki, D. Tanaka, K. Okamoto, K. TAMADA
- 1375.** Development of surface enhancing Raman scattering biosensing platform with graphene hybrid nanocomposite and DNA aptamers. A. Mahmoud, M. McDermott*
- 1376.** Enhanced two-photon absorption behavior of acetylenic compounds obtained by the confinement in the interlayer space of inorganic nanosheets. M. Tominaga, H. Sugihara, S. Mochida, K. Satomi, Y. Suzuki, J. Kawamata*
- 1377.** Clay minerals incorporating metal complexes for colorimetric solvent and humidity indicators. H. Hosokawa, T. Mochida*
- 1378.** How reactive are supramolecular azobenzene moiety in nanolayered microenvironment. S. Hassan, V. Ramakrishnan, H. Horiguchi, D. Yamamoto, Y. Nabetani*, H. Tachibana, H. Inoue*
- 1379.** Formation of vortex-shaped orientation of niobate oxide nanosheet liquid crystals by irradiation of an optical vortex. T. Sakurai, R. Nakanishi, M. Tominaga, Y. Suzuki, J. Kawamata*, Y. Shimura, T. Iwai, Y. Nono, T. Nakato
- 1380.** Orientation of niobate oxide nanosheet liquid crystals under circularly polarized laser beam. R. Nakanishi, M. Tominaga, Y. Suzuki, J. Kawamata*, Y. Shimura, T. Iwai, Y. Nono, T. Nakato
- 1381.** Theoretical study of the thermoelectric property of phosphorene under the tensile strain. S. Konabe*, T. Yamamoto
- 1382.** Thermal behavior of adsorbed water and electrolyte solution in clay minerals. Y. Ito, A. Nagoe, T. Sugimoto, H. Fujimori, T. Takemura
- 1383.** Multiphase coexistence of liquid crystalline phases in binary colloids containing inorganic nanosheets. E. Moura, M. Nakashima, T. Nakato
- Hawaii Convention Center
Halls I, II, III
- Applications of Ultrasound to Nanoscience (#150)**
- Organized by: K. Suslick, F. Grieser, M. Atobe, J. Yu, S. Jeong
- Poster Session**
19:00 – 21:00
- 1384.** Measurement of sound pressure under cavitation conditions. Y. Asakura*, T.T. Nguyen, K. Yasuda, S. Koda
- 1385.** Microbubble generation from gas supersaturated water by ultrasonic stimulation. K. Terasaka*, I. Yamazaki, S. Fujioka
- 1386.** Ultrasonic effect on nano- and micro-particles, microbubbles, and fluid flow in microspace and its application to a microreactor. Z. Ekaputra
- 1387.** Sonochemical synthesis of Au nanoparticles onto iron-based cathode materials for lithium ion battery. Y. Ono*, H. Okawa, K. Sugawara
- 1388.** Ultrasound-assisted growth of hydroxyapatite films on magnesium alloy AZ31. C. Liu*, A. Keller, G. Grundmeier
- 1389.** Metal nanoparticles synthesis onto cathode materials for lithium ion battery using sonochemical method. H. Okawa*, Y. Ono, M. Takai, K. Uematsu, K. Sugawara, M. Sato
- Hawaii Convention Center
Halls I, II, III
- Carbon Nanotubes: Preparation, Characterization and Applications (#227)**
- Organized by: S. Maruyama, R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: S. Maruyama, R. Xiang
- Poster Session**
19:00 – 21:00
- 1390.** Understanding surfactant structure at the surface of carbon nanotube via single molecule fluorescence spectroscopy. R. Pramanik, S.K. Doorn, J. Duque
- 1391.** Influence of covalent dopants on the optical properties and exciton lifetimes in single-wall carbon nanotubes. N.F. Hartmann*, X. Ma, E.H. Házor, S. Yalcin, H. Htoon, S.K. Doorn
- 1392.** Using supercritical carbon dioxide to create multiscale composites. D.G. Baird*
- 1393.** Dielectric/electric properties of composites filled with multiwalled carbon nanotubes. J. Banys*, I. Kraunauskaitė*, J. Macutkevič, V.L. Kuznetsov, S. Moseenkov
- 1394.** Efficient semiconducting single-walled carbon nanotube sorting with a removable solubilizer based on dynamic supramolecular chemistry. N. Nakashima*, F. Toshimitsu
- 1395.** Characteristics of polybutylene terephthalate composites containing polybutylene terephthalate grafted multi-walled carbon nanotubes fabricated by reactive extrusion. E. Choi*, J. Kim, Y. Jo, c. Kim
- 1396.** Atmospheric-pressure controllable synthesis of heteroatom-doped carbon nanotube and its applications for electrochemical energy storage and conversion. W. Chiang*, M. Yeh, T. Li, L. Lin, Y. Leu, Y. Li, G. Chen, K. Ho
- 1397.** Alteration of blend morphology via the addition of long nanotubes. B. Brady*, S. Crossley, J. Guo, J. Zapata, N. Briggs
- 1398.** In situ observation of intermediates in chemical vapor deposition synthesis of carbon nanotube. S. Inoue*, Y. Ohga, Y. Matsumura
- 1399.** Carbon nanotube electrodes for vanadium redox flow batteries. K. Iseki, G. Oriji, M. Ichikawa, K. Hanawa
- 1400.** Preparation of Poly(*N*-isopropylacrylamide) terminated carbon nanotubes and their aggregation properties responding to infrared light and heating. R. Ishizaki, S. Tamesue, T. Mitsumata, N. Tsubokawa, T. Yamachi*
- 1401.** Organic and elemental molecules encapsulated in single-walled carbon nanotubes as Na and Li ion battery electrodes. S. Kawasaki, Y. Ishii, Y. Sakamoto
- 1402.** Synthesis and characterization of Co nanoparticles on multiwall carbon nanotubes for catalytic applications. M.A. Kazakova*, A.S. Andreev, A.V. Ishchenko, O.B. Lapina, V.L. Kuznetsov
- 1403.** Artificial muscle response to temperature. H. Kim, R.H. Baughman*, S. Kim*
- 1404.** Effect of chirality separation on SW-CNT-TFTs using DNA-wrapped SW-CNTs. Y. Kuwahara*, F. Nihey, S. Ohmori, T. Saito
- 1405.** Water adsorption phenomena on vertically-aligned single-walled carbon nanotubes. J. Kuwahara, S. Chiashi, G. Yamaguchi, H. Kato, Y. Homma
- 1406.** Extraordinary mechanical flexibility of bimetallic AgPt nanoparticle-decorated carbon nanotubes on PET substrates. K. Lin*
- 1407.** Construction of unique logic circuits using carbon-nanotube-composite papers. K. Matsui*, T. Oya
- 1408.** Development of paint-type dye-sensitized solar cell using carbon nanotube paint and its evaluation. Y. Matsunaga*, T. Oya
- 1409.** Tight binding models of carbon nanotube and applications to quantum information processing. M. McGuigan*
- 1410.** Thermoelectric properties of single-walled carbon nanotubes filled in ionic liquid polymers. M. Nakano*, Y. Nonoguchi, T. Nakashima, T. Kawai
- 1411.** Organic thermoelectric hybrid of inorganic 1D nanomaterials and conducting polymer or polymer complex. K. Oshima*, Y. Shiraiishi, N. Toshima
- 1412.** Yarn-based enzymatic biofuel cell for biomedical applications. Y. Park, R.H. Baughman*, S. Kim*
- 1413.** Structure and properties of chalcogen encapsulated carbon nanotubes studied by molecular dynamics simulations. Y. Sato*, Y. Kataoka, H. Ogata
- 1414.** Fluid dynamic slicing of super tensile carbon nanotubes. K. Vimalanathan*, J. Gascooke, H. Kumar, M. Lawrence, J.L. Atwood, C. Raston
- 1415.** Single-walled carbon nanotubes as etching masks for ion sputtering. W. Yim, H. Jeong, S. Park, Y. Ahn, S. Lee, J. Park*

* Principle Author

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1416. Local structures and properties of the alkali halide crystals encapsulated in single-walled carbon nanotubes studied by molecular dynamics simulations and solid-state NMR. **E. Yokokura**, **Y. Kataoka**, **H. Ogata**

1417. Toward roll-to-roll production of carbon nanotubes using microwave. **X. Zhang***, **J. Cook**

Hawaii Convention Center
Halls I, II, III

Self-organization of Membrane Systems (#259)

Organized by: D. Sasaki, K. Morigaki, I. Kooper

Presiding: D. Sasaki

Poster Session

19:00 – 21:00

1418. Solid-state NMR and microscopic studies of synthetic mimic of GPI-anchored proteins. **K. Nomura**, **E. Harada**, **K. Sugase**, **K. Shimamoto**, **F. Hayashi**, **K. Morigaki**

1419. Distribution and orientation of voltage-dependent K⁺ channel KAT1 reconstructed to ascorbin supported lipid bilayer observed with atomic force microscope. **Y. Suzuki***, **A. Nozawa**, **Y. Tozawa**, **R. Tero**

1420. Mimicry of membrane curvature sensing proteins by polymethacrylate random copolymers. **M. Tsukamoto***, **J. Kikuchi**, **K. Kuroda**, **K. Yasuhara**

1421. Reconstitution of Min system in artificial cells. **S. Kouyama**, **K. Fujiwara**, **N. Doi**

1422. Substrate-dependent asymmetric and anisotropic diffusion in supported lipid membrane. **T. Motegi***, **K. Yamazaki**, **T. Ogino**, **R. Tero**

1423. Fluidity evaluation of supported lipid bilayer prepared on graphene oxide based on single particle tracking. **Y. Okamoto**, **T. Motegi**, **S. Iwasa**, **A. Sandhu**, **R. Tero***

1424. Selective partitioning to the liquid ordered phase: Fluorescent lipid probes. **D. Sasaki***, **J. Stachowiak**, **G.D. Bachand**

1425. Liposome-based liquid handling for biochemical reactions. **T. Okano**, **H. Suzuki**, **T. Yomo***

1426. Membrane interactions of the PTEN tumor suppressor and the conundrum of dominant-negative mutations. **M. Lüsche***, **F. Heinrich**, **A. Gericke**, **R. Harishchandra**, **H. Nanda**, **A. Ross**

1427. Significance of charged lipids in tuning the dynamic properties of biomembranes. **E.G. Kelley**, **A.C. Woodcock**, **K. Wood**, **P.D. Butler**, **M. Nagao**

1428. L-proline catalyzed Michael addition reaction conducted at liposome interface. **M. Hirose**, **T. Ishigami**, **K. Suga**, **Y. Okamoto**, **H. Umakoshi***

1429. 2D structure of supported lipid bilayer reconstructed with human *ether-a-go-go*-related gene channel. **K. Fukumoto**, **Y. Ishinari**, **A. Hirano-Iwata**, **M. Niwano**, **R. Tero**

1430. Engineering nanoscopic features within solid-supported membrane. **J. Kurniawan**, **J. Ventrici**, **G. Liu**, **T. Kuhl**

1431. COOH modification of SiO₂/G.Si surface with water-soluble silane coupling agent. **Y. Niizuma***, **N. Misawa**, **R. Tero***

1432. Preparation of lipid membrane supported by structured porous materials as a multicellular biomembrane model. **K. Ueno**, **K. Matsumura***

1433. Nanometal gap structure for the selective transport and detection of biological molecules. **K. Ando***, **M. Tanabe**, **K. Morigaki**

1434. Evaluating the raftophilicity of rhodopsin in a patterned model membrane. **Y. Tanimoto**, **F. Hayashi**, **K. Morigaki**

Hawaii Convention Center
Halls I, II, III

Membranes and Nanotechnologies for Energy and Environment Applications (#317)

Organized by: H. Park, B. Freeman, B. McCloskey, J. McGrath, A. Hill, A. Higuchi, Y. Lee

Poster Session

19:00 – 21:00

1435. Preparation of functional membrane materials by assembly of polymer brush nanoparticles. **I. Zharov**

1436. Mixed matrix membranes based on poly(trimethyl silyl propyne) (PTMSP) and graphene-based nanoplatelets with reduced ageing and modified permselectivity. **L. Olivieri**, **S. Ligi**, **M. De Angelis**

1437. Highly ion conductive perfluorinated sulfonic acid ionomer reinforced membranes for energy generation and valued chemicals production. **S. Kang**, **E. Jeon**, **I. Park**, **Y. Goo**, **J. Park**, **Y. Cho**, **J. Shim**, **J. Lee**, **D. Lee**, **C. Lee***

1438. Fluidic active transducer for electricity generation. **Y. Yang**, **J. Park**, **S. Chung**, **Y. Ahn**, **Y. Kim***

1439. Novel concept for the design of block copolymer membranes via a modular chemical ligation approach. **M. Langer**, **C. Hörenz**, **C. Pietsch**, **A. Goldmann**, **F.H. Schacher**, **C. Barner-Kowollik***

1440. Simple spray coating method to prepare superhydrophobic teflon/Al₂O₃ membrane for desalination applications. **C. Huang**, **H. Chiu**, **Y. Liao***

1441. Synthesis, characterization, and alkaline stabilities of graft-type anion conducting electrolyte membranes containing Poly(4-vinylimidazolium) grafts and application to alkaline fuel cells. **S. Watanabe***, **K. Yoshimura**, **T. Hagiwara**, **Y. Maekawa**

1442. Molecular dynamics simulation study of cation exchange membrane for electrodosorption-deionization method. **T. Son**, **C. Park**, **E. Tocci**, **S. Nam***

1443. Preparation and characterization of ultrafiltration hollow fiber membrane for drinking water. **S. Woo**, **S. Nam**

1444. Proton transport property in organized polyimide thin films. **Y. Ono**, **S. Tsuyuki**, **M. Hara**, **S. Nagano**, **Y. Nagao***

1445. Colorimetric solvent indicator based on Nafion films incorporating metal complexes. **H. Hosokawa**, **Y. Funasako**, **T. Mochida***

1446. Origin of CO₂-philicity in graphene oxide membranes. **H. Yoon***, **H. Kim**, **J. Shin**, **B. Yoo**, **H. Park**

1447. Visualization of concentration polarization of nanoparticles during crossflow membrane ultrafiltration using the laser-induced fluorescence (LIF) technique. **B. Meng***, **P. Liu**, **X. Li**

1448. Detection of TNT and RDX based on gold nanoparticles molecular imprinted matrix by surface plasmon resonance and surface-enhanced Raman spectroscopy. **G. Granger***, **T. Brulé**, **N. Bukan**, **M. Vidal**, **J. Masson**

1449. Electrospun nanofiber absorbents for uranium extraction from seawater. **J. Li**

1450. Characteristics of ultrafiltration membranes fabricated from amine terminated polyethersulfone and self-assembled zinc oxide nanoparticles on the membrane surface. **Y. Jo***, **E. Choi**, **J. Kim**, **C. Kim**

1451. Innovative sPEEK nanocomposites by nanoparticles with external protons. **S. Kim**, **H. Rhee***, **T. Yun**, **S. Choi**

1452. Tuning gas transport properties of graphene-based membranes by inserting coronene and its derivatives. **B. Yoo***, **S. Jang**, **J. Shin**, **H. Park**

1453. Composite anion exchange membrane based on cellulose crosslinked polysulfone for application in urea based fuel cell. **G. Das**, **D. Kim**, **K.H. Kim**, **H.W. Choi**, **H. Hee Yoon***

1454. Improvement of cyclohexene yield in cyclohexane dehydrogenation or benzene dehydrogenation by a pore-through catalytic reactor. **M. Hasegawa**, **T. Sato**, **N. Itoh***

1455. Vacuum membrane desiccant cooling for personal heat stress management. **y. yang**, **c. lan***

1456. Synthesis of hydrophilic zeolite membranes and their dehydration performance for alcohol – water mixture. **Y. Kikuchi**, **T. Sato**, **N. Itoh***

1457. Gas separation properties of composite membrane based on PDMS graft co-polyimide coated with nanosheet of PEO graft copolyamide. **K. Ando**, **A. Abeta**, **Y. Okamura**, **Y. Nagase***

1458. Forward osmosis nanochannel membrane for seawater desalination. **S. Choi**

1459. Development of innovative reverse osmosis membranes for desalination. **H. Shirama***, **K. Nakatsui**, **T. Sasaki**, **M. Kimura**

1460. Enhanced pervaporation dehydration of acetone by using polyimide membranes modified by novel vapor phase crosslinking and tripodal amine crosslinking. **D.W. Mangindaan***

1461. Hydrophilic-surface modified CNT-embedded thin-film polyamide membrane and its 8-inch spiral wound module performance. **H. Lee***, **J. Seon**, **M. Kim**, **B. Michael**, **J. Kim**, **H. Park**

1462. Improvement of separation property of PDMS graft polyimide membrane by nanosheet coating of polymers containing imidazolium group. **T. Oda**, **K. Taira**, **M. Watanabe**, **S. Koguchi**, **Y. Okamura**, **Y. Nagase***

1463. High-flux graphene oxide thin-film composite membranes for CO₂ separation. **M. Yoo**, **H. Park**, **J. Shin**, **S. Jang**, **H. Yoon**

1464. Gas permeation properties of poly(sulfone-co-ethylene glycol) membranes containing bis(phenyl)fluorene groups. **D. Kim***, **H. Lee**, **S. Nam**

1465. Oil-water separation by a titanium dioxide filter with self-cleaning property. **S. Nishimoto**, **M. Ota**, **Y. Kameshima**, **M. Miyake**

1466. Pervaporation and vapor permeation performance of hollow-fiber carbon membranes for the dehydration of organic solvents. **M. Yoshimune***, **N. Hara**, **K. Haraya**

1467. Long-term stability of graphene oxide thin-film composite membranes: Effect of temperature and humidity. **J. Shin**, **H. Yoon**, **J. Park**, **M. Yoo**, **B. Yoo**, **B. Freeman**, **H. Park**

1468. Facile methodology for the production of in-situ inorganic nanowire hydrogels/aerogels and their environmental applications. **H. Jung***, **S. Jung***, **J. Kong**

1469. Graphene oxide membranes for water purification and desalination applications. **Y. Cho**, **J. Shin**, **S. Jang**, **B. Yoo**, **H. Park***

Hawaii Convention Center
Halls I, II, III

Ceramic Materials and Processing for Advanced Applications (#341)

Organized by: F. Rosei, A. Vomiero, Y. Tachibana, C. Raston, H. Zhang

Poster Session

19:00 – 21:00

1470. Simultaneous 3D printing of calcium phosphate and osteoblast-laden hydrogel for bone tissue regeneration. **H. Yun***, **R. Naren**

1471. Fabrication of strontium fluoroapatite ceramics by reactive-templated grain growth method using hexagonal-shaped tristrontium phosphate particles. **A. Ishida**, **A. Suzumura**, **Y. Kishida**, **T. Tani**, **M. Aizawa***

1472. Synthesis of a nitrogen-containing carbon material with oxygen reduction activity from polymer precursors. **A. Idesaki***, **M. Sugimoto**, **A. Shimada**, **S. Yamamoto**, **M. Taguchi**, **T. Yamaki**

1473. Systematic color control of a, β-FeOOH nano pigments by adjusting size and shapes depending on pH synthetic conditions. **I. Kim***, **R. Yu**, **J. Yun**, **Y. Kim***, **E. Choi***

1474. Synthesis of chiral TiO₂ employing soft catalytic template containing polyethyl-enimine/tartrate. **K. Murakami**, **H. Matsukizono**, **M. Saito**, **R. Jin**

1475. Preparation of SnO₂ thin films with a non-equilibrium 2D plasma at room temperature under atmospheric pressure. **Y. Masuda***, **S. Kanezashi**, **M. Tan**, **M. Okuya**

1476. TiO₂ thin films prepared with a non-equilibrium 2D plasma induced by a surface discharge technique at room temperature. **Y. Masuda***, **M. Tan**, **S. Kanezashi**, **M. Okuya**

1477. Synthesis of the porous Si from rice husk ash (SiO₂) using magnesium reduction method in a fluidized bed. **W. Cho**, **M. Seo**, **H. Ra**, **J. Lee**, **H. Lee**

1478. Study of phase transitions between γ-Ti₂O₅ and δ-Ti₂O₅. **T. Nasu**, **K. Tanaka**, **Y. Miyamoto**, **N. Ozaki**, **S. Tanaka**, **T. Nagata**, **F. Hakoe**, **M. Yoshiyuki**, **K. Nakagawa**, **Y. Umetsu**, **K. Imoto**, **H. Tokoro**, **A. Namai**, **S. Ohkoshi**

1479. Synthesis of disk-like cross-linked polyamines gels with crystalline domain and their activity in silica deposition. **D. Soma**, **R. Jin**

1480. Chromogenie mechanism of Aka-e, a red overglaze enamel decoration on porcelain body, created with lead-free glazes and hematite particles. **H. Inada***, **H. Hashimoto**, **Y. Okazaki**, **Y. Arakawa**, **T. Takaishi**, **H. Taguchi**, **S. Hashida**, **T. Fujii**, **J. Takada**

1481. Microwave absorption properties of the mechanically surface treated alumina powders and their hydration behavior. **T. Shirai***, **M. Fuji**

1482. Novel 3D printing process of calcium phosphate scaffolds for bone tissue regeneration. **H. Yun***, **G. Tripathi**

1483. Synthesis and characterization of cat-ionic conductive aluminum tungstates. **A. Ueyama***, **R. Shimanouchi**

1484. Influence of alcohol addition to hydrothermal synthesis of NASICON-type mixed valent solid solutions, Na_{1+x}Ti_{2-y}Fe_y(PO₄)₃. **T. Kurosaka***, **R. Shimanouchi**

1485. New durable bulk material of NaSn₂(PO₄)₃ synthesized by low temperature calcination of hydrothermally prepared sols. **R. Shimanouchi**, **A. Ueyama**, **T. Kurosaka**

1486. Crystallization kinetics and phase transformation of lithium aluminosilicate glass in heating process. **N. Mishima***, **T. Matsumoto**, **M. Nakamura**

1487. Application of kaolinite ceramics granules to hemodialysis water. **K. SATO***, **T. MURAKAMI**, **T. UJIHARA**, **K. OKAJIMA**, **T. IMOTO**, **A. MORI**, **M. MURAMATSU**

1488. Fabrication of visible light responsive N-doped TiO₂ coating through anodic oxidation process. **K. Yokoi***, **N. Ohtsu**

1489. Crystal growth of Cu-substituted Mayenite single crystals by the FZ method using the mirror-tilted type furnace. **E. Maruyama***, **M. Nagao**, **S. Watauchi**, **I. Tanaka**

1490. Crystal structure and luminescence of Lu₃Al₅O₁₂ doped with Ce³⁺ and N³⁻. **W. Ahn**, **Y. Kim***

1491. Photocatalytic property of PbTiO₃/TiO₂ heterostructured nanotube. **H. Kim**, **C. Ahn**, **K. Hong**

* Principle Author

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Design of Innovative Photochromic Applications (#399)

Organized by: J. Abe, T. Kawai, Y. Yokoyama, N. Branda, F. Raymo, W. Zhu

Poster Session
19:00 – 21:00

1492. Comparative investigation of photochromism of spironaphthooxazine in nanoparticle colloid, bulk solid, and solution. Y. Ogura, Y. Ishibashi, **T. Asahi***

1493. Photo-induced fluorescence switching property of single diarylethene derivatives. **S. Ito**, T. Ikegami, Y. Arai, H. Miyasaka, K. Uno, Y. Takagi, M. Morimoto, M. Irie

1494. Cooperative fluorescence color changes of a dibenzylmethane boron complex during the molecular assembling process. **F. Ito***, Y. Suzuki, J. Fujimori, T. Sagawa

1495. Multiphoton cycloreversion reaction of diarylethene nanoparticles. **Y. Ishibashi***, Y. Ogura, H. Miyasaka, T. Asahi

1496. Reversible photochemical reactions in a flexible crystalline nanospace. **H. Sato***, Y. Zheng, S. Kitagawa

1497. Synthesis of dithienylethenes and their application in sensing technology. **G. Vamvounis**, D. Gendron

1498. Photocontrol of 2D self-assembly of photochromic molecules at liquid/solid interface. S. Yokoyama, T. Hirose, **K. Matsuda***

1499. Visible light-driven photocatalyst with gold nanoparticle two-dimensional arrays as a high intense field light source. **K. Isozaki***, F. Pincella, K. Miki*

1500. Photoinduced mass transport observed for azobenzene-based photochromic amorphous molecular materials. **H. Nakano***, M. Suzuki, R. Ichikawa, R. Matsui, R. Ichikawa

1501. Structural dynamics in azobenzene liquid crystal polymer films studied by microscopic and time-resolved techniques. **K. Katayama**, S. Kuwahara, T. Ikeda

1502. Chiral molecular photoswitches containing a binaphthyl unit. **T. Ubukata***, M. Samata, R. Kato, Y. Takei, Y. Yokoyama

1503. Conversion of light into macroscopic motion in spiropyran containing LC polymer films. **T. Yamaguchi***, S. lamasaard, N. Katsonis*

1504. Coordination-driven control of photoisomerization behavior of macrocyclic azobenzene. **M. Yamamura**, T. Nabeshima

1505. Mechanism of photo-induced nano-sheet sliding on azobenzene/niobate hybrids. **Y. Nabetani***, H. Horiguchi, S. Matsukura, S. Hassan, V. Ramakrishnan, H. Tachibana, H. Inoue*

1506. Photochromism and photoinduced mass transport of naphthacenequinone compounds. **M. Moriyama***, S. Kai, T. Ueshima, N. Kawano, A. Takagaki, Y. Abe, H. Shin, T. Takeshima, K. Mukai, S. Nagano, T. Seki

1507. Two-photon-gated photochemical reaction in [2.2]paracyclophane-bridged bis(imidazole dimer). **K. Mutoh**, Y. Nakagawa, I. Yonekawa, A. Tsuchiya, A. Sakamoto, Y. Kobayashi, J. Abe*

1508. CB[8] gated photochromism of a diarylethene derivative containing thiazole orange groups. **Y. Mao**, K. Liu, T. Yi

1509. UV light irradiation wavelength dependence on the photoinduced bending behavior of photochromic diarylethene crystals. **D. Kitagawa**, S. Kobatake*

1510. Quinone based diarylenes for near IR initiated photoisomerization. **D. Carter***, D.G. Patel, F. Novak, S. Myers

1511. Photochromic reactions of spirooxazines and spiropyrans having a hydroxyphenyl group. H. Tago, **T. Nakagawa***, Y. Yokoyama

1512. Synthesis and characterization of amphiphilic silica nanoparticles covered with block copolymers branching photocromatic diarylethene moieties on side chain. **K. Shimizu**, R. Seno, S. Kobatake*

1513. Enantioselective photocyclization of diarylethene incorporated in human serum albumin. **Y. Watanobe***, K. Osawa, K. Kawamura, T. Nakagawa, Y. Yokoyama

1514. Photochromic phenoxyl-imidazolyl radical complexes with decoration rates tens of nanoseconds to seconds. **H. Yamashita**, T. Ikezawa, Y. Lee, Y. Kobayashi, J. Abe

1515. Photoinduced formation/disappearance of 2D ordering of 2-thienyl-type diarylethane at the solid/liquid interface: A cooperative self-assembly process. **S. Yokoyama**, T. Hirose, K. Matsuda*

1516. Photoconversion of pentacenedi-*k*-one derivative in the crystalline phase: Shape change of single crystals during the photoconversion. **Y. Miyamoto***, M. Suzuki, N. Aratani, H. Yamada, S. Masuo

1517. Photoresponsive magnetic nanoparticle composed of spiropyran and FePt. **K. Tsuda***, T. Hosomi, E. Yuryeva, T. Yamamoto, Y. Einaga

1518. Photoionization of diarylethene included cyclodextrin using multicolor multilaser irradiation. **T. Takeshita**, M. Hara, Y. Kasaba

1519. Photoinduced topographical changes of surfaces of diarylethene derivatives with pyridinium salts. **K. Takase**, Y. Kojima, M. Morimoto, S. Yokojima, S. Nakamura, K. Uchida*

1520. Fluorescence photoswitching of diarylethene derivatives: A single-molecule study. **T. Ikegami***, S. Ito, H. Miyasaka, K. Uno, Y. Takagi, M. Morimoto, M. Irie

1521. Modulation of fluorescence character of diarylethene. **S. Takeuchi***, T. Nakagawa, Y. Yokoyama

1522. Photoswitching of intramolecular π -stacking. **Y. Hashimoto**, T. Nakashima, T. Kawai*

1523. Photochemical control of vesicle formation in an aqueous mixture of a photo-switchable cationic surfactant modified with cinnamic acid and an anionic surfactant. **K. Hattori**, M. Akamatsu, K. Tsuchiya, T. Endo, K. Torioge, K. Sakai, M. Abe, H. Sakai*

1524. Synthesis and optical properties of novel phenoxyl: Imidazolyl radical complex derivatives. **Y. Mishima**, H. Yamashita, Y. Kobayashi, Y. Yoneda, T. Katayama, H. Miyasaka, J. Abe

1525. Synthesis and photochemical properties of pentaarylimidazole derivative substituting pyrenyl groups. **D. Ozeki**, H. Yamashita, Y. Kobayashi, J. Abe

1526. Photoformation of surface relief grating on photopolymerizable bisanthracene films. **T. Sonoda**, M. Nakayama, H. Kihara, T. Ubukata*

1527. Excitation wavelength dependence of photochromic reaction of diarylethene derivatives: Correlation between reaction quantum yields and femtosecond dynamics. **K. Ume**, T. Katayama, H. Miyasaka, S. Kobatake, M. Irie

1528. Reversible photoinduced linear birefringence change of diarylethene single crystals. **H. Tsujioka**, S. Kobatake*

1529. Photochromic and fluorescent properties in push-pull terarylene systems. **R. Kanazawa**, T. Nakashima, M. Sliwa, S. Delbaere, T. Kawai*

1530. Synthesis and photochromic properties of diarylenes having a benzophenone group. **T. Ichikawa**, M. Morimoto, M. Irie

1531. Single-molecule tracking of photo-switchable fluorescent diarylethene derivatives in polymer thin films. **Y. Arai***, S. Takei, S. Ito, H. Miyasaka, K. Uno, Y. Takagi, M. Morimoto, M. Irie

1532. Optical properties of an azobenzene-bridged imidazole dimer. **H. Arai**, K. Mutoh, Y. Kobayashi, J. Abe*

1533. Development of a photochromic phenoxyl-imidazolyl radical complexes having thiophene backbone. **T. Ikezawa**, K. Mutoh, H. Yamashita, Y. Kobayashi, J. Abe

1534. Photochromic properties of biphenyl-bridged imidazole dimers by changing distances between two cross-linking points. **Y. Fujita**, H. Yamashita, Y. Kobayashi, J. Abe

1535. Revealing the initial process of the photochromic reaction of biphenyl-bridged imidazole dimer. **T. Yamaguchi**, M.F. Hilbers, P.P. Reinders, Y. Kobayashi, A.M. Brouwer, J. Abe*

Hawaii Convention Center
Halls I, II, III

Advances in Organic Light-Emitting Diodes (#409)

Organized by: J. Bredas, C. Adachi, K. Wong, V. Yam, P. Burn, J. Kim

Poster Session
19:00 – 21:00

1536. Molecular diffusion during formation of interfaces containing small molecules from solution process for organic light-emitting devices. **S. Ohisa***, Y. Pu, N. Yamada, G. Matsuba, J. Kido

1537. Development of solution-processable dendritic thermally activated delayed-fluorescence materials. **K. Albrecht**, K. Matsuka, K. Fujita, K. Yamamoto*

1538. Hydrocarbon macrocycles for organic-light emitting devices. **S. Sato***, J.Y. Xue, T. Izumi, A. Yoshii, K. Ikemoto, T. Koretsune, R. Akashi, R. Arita, H. Taka, H. Kita, H. Isobe

1539. Triplet recombination dynamics: Role of interfacial order and state delocalization. **E.R. Bittner**

1540. Direct investigation of the excited-state dynamics of thermally-activated delayed fluorescence molecules: Pump-probe transient absorption spectroscopy. **T. Hosokai***, H. Matsuzaki, A. Furube, K. Tokumaru, T. Tsutsui, H. Nakanotani, M. Yohiro, C. Adachi

1541. Photoluminescence of liquid-crystalline gold complexes with a biphenyl mesogenic core. **Y. Rokusha**, S. Yamada, O. Tsutsumi*

1542. Electron conducting properties of luminescent gold complexes. **H. Nakasato**, S. Shimai, S. Yamada, O. Tsutsumi*

1543. Synthesis and characterization of the new emitters for OLED applications. **R. Lygaits***, O. Zeika, R. Scholz, P. Kleine, F. Wüst, M. Oberländer, S. Hofmann, J.V. Grzalevicius, S. Reineke

1544. Radiative transition of conjugated organic molecular aggregates: A theoretical investigation with all normal vibrational modes. **W. Li**, L. Zhu, Q. Peng, Z. Shuai

1545. Orientation of phosphorescent emitting dipoles for highly efficient organic light-emitting diodes. **K. Kim**, C. Moon, J. Kim*

1546. Structurally robust phosphorescent $[Pt(O^{\bullet}N^{\bullet}C^{\bullet}N)]$ emitters for high performance organic light-emitting devices with power efficiency up to 126 lmW^{-1} and external quantum efficiency over 20%. **A. Wai Hung**

1547. Structurally robust phosphorescent $[Pt(O^{\bullet}N^{\bullet}C^{\bullet}N)]$ emitters for high performance organic light-emitting devices with power efficiency up to 126 lmW^{-1} and external quantum efficiency over 20%. **M. Ko**

1548. Theoretical study on radiationless decay rate of molecular aggregates based on split-operator method. **L. Zhu**, Q. Peng, W. Li, Z. Shuai*

1549. Solution processed small molecule doped white light emitting diode based on a new polyfluorene copolymer. **P.K. Iyer**, D. Das*, P. Gopikrishna, A. Dey, A. Singh, R. Narasimhan

1550. Efficient red electroluminescent devices with sterically hindered phosphorescent platinum(II) Schiff-base complexes and with iridium complex co-dopant. **C. Kwong**, L. Zhou, C. Kwok, G. Cheng, H. Zhang, C. Che*

1551. Hybrid OLEDs with CdS_xSe_{1-x}/ZnS core-shell type quantum dot layers: An investigation of electroluminescence properties. **B.L. Vasilauskienė**, M. Vitkus, G. Juska, K. Genievicius

1552. Introducing a thermally activated delayed fluorescence emitter for a highly efficient blue fluorescent organic light emitting diode. **J. Sun**, Y. Kim, J. Kim*

1553. Photophysical studies of the thermally activated delayed fluorescence from efficient organic light-emitting diodes. **D. Kim**, H. Shin, T. Ahn*

1554. DNA-guided organic light-emitting materials enabling biospecificity. **J. Park**, S. Paik, C. Cui, D. Ahn*, J. Cho

1555. Spiro-based ecofriendly green semiconductors for OLEDs. **L. Xie***, Y. Wei, X. Zhang, W. Huang*

1556. Temperature distribution measurements of large-area organic light-emitting diodes by Raman spectroscopy.

T. Yokoyama*, Y. Furukawa, K. Katagi, H. Ohata, S. Miyaguchi, T. Tsutsui

1557. Raman study of hole accumulation at NPD/Alq₃ interfaces of fresh and aged organic light-emitting diodes. **Y. Karatsu**, Y. Furukawa, T. Miyamae, H. Okumoto, T. Tsutsui

1558. Suppression of nonradiative decay from triplet excited state by weak intermolecular interactions. **R. Kabe**, N. Notuka, C. Adachi*

1559. Study of intramolecular relaxation processes of thermally activated delayed fluorescence materials for suppressing external quantum efficiency roll-off in organic light-emitting diodes. **M. Inoue***, T. Serevičius, H. Nakamoto, K. Yoshida, T. Matsushima, C. Adachi

1560. Exciton quenching analysis of thermally activated delayed fluorescence molecules by time-resolved photoluminescence measurement.

A.S. Sandanayaka*, K. Yoshida, T. Matsushima, C. Adachi

1561. Improvement of electrical properties of organic films by cold isostatic pressing.

Y. Esaki*, T. Matsushima, C. Adachi

1562. Organic light-emitting diodes combining emission from both monomeric and exciplex excitons based on aggregation-induced derivatives of carbazole and tetra(4-phenyl)ethylene. **A. Tomkeviciene**, J. Sutaite, D. Volyniuk, J.V. Grzalevicius

1563. Inverted organic light-emitting diodes utilizing zinc oxide based transparent conductive films. **M. Takada***, T. Kobayashi, T. Nagase, H. Naito*

1564. Long-lived phosphorescence based organic light emitting diodes.

N. Notuka, R. Kabe, C. Adachi*

1565. Synthesis and optical properties of fluorene derivatives bearing S,S-dioxidized thiophene. **T. Nakahama**, S. Kobatake*

1566. Dual enhancement of electroluminescence efficiency and operational stability by rapid utilization of triplet excitons for light emission. **T. Furukawa**, H. Nakanotani, C. Adachi

1567. Conservation laws, radiative decay rates, and excited state localization in organometallic complexes with strong spin-orbit coupling. **B. Powell***

* Principle Author

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1568. High efficiency blue organic light emitting diodes using thermally activated delayed fluorescence. **h. noda**, R. Kabe, C. Adachi

1569. Nano-structured organic light emitting diode for suppression of roll-off characteristics toward electrically-pumped organic semiconductor laser diodes.

H. Kuwae*, A. Nitta, T. Kasahara, K. Yoshida, S. Shoji, C. Adachi, J. Mizuno
1570. Enhancement of light out-coupling efficiency for organic light-emitting diodes. **S. Kubo**, K. Suzuki, T. Fukushima, H. Kaji*

1571. Electron coupling and disorder in organic semiconductors. **S.R. Kimura**, D. Yoshidome, J.L. Gavartin, A. Goldberg, M.D. Halls, D. Giesen

1572. Highly efficient solution-processed organic light-emitting diodes using thermally activated delayed fluorescence. **Y. Wada**, K. Shizu, K. Suzuki, S. Kubo, H. Tanaka, C. Adachi, H. Kaji*

1573. Novel bis(phenylbenzothiadiazole derivatives as highly efficient solution-processed non-doped red light-emitting materials for OLEDs. **V. Promarak***

1574. Operational lifetime enhancement in TADF OLEDs. **P.D. Tsang**, C. Adachi

1575. Improved efficiency roll-off and lifetime for hybrid white organic light-emitting diodes using triplet harvesting system. **S. Lee***, H. Lee, J. Lee, S. Yoon, Y. Kim

1576. Syntheses and physical properties of carbazole-phthalonitrile-hybridized light-emitting materials. **A. Orta**, K. Shinohara, Y. Suzuma, T. Nishida, J. Otera

1577. Study on stable emission of ruthenium complex for light-emitting electrochemical transistor. **M. Nakano***, A. Aoki

1578. Preparation and evaluation of iridium complex for light-emitting electrochemical cell. **T. Kubo***, A. Aoki

1579. Organic light-emitting diodes exploiting thermally activated delayed fluorescence: Development of a new emitter material and the analysis. **H. Kaji***, H. Suzuki, T. Fukushima, K. Shizu, K. Suzuki, S. Kubo, T. Komino, H. Oiwa, F. Suzuki, A. Wakamiya, Y. Murata, C. Adachi

1580. Conjugation-extended fluorene derivatives for OLEDs. **H.P. Rathnayake**, A. Cirpan, F.E. Karasz, **P.M. Lathi**

1581. Solution-processable small molecule-based emitting layers for multicolor OLEDs. **S. Olivier**, L. Derue, B. Geffroy, T. Maingron, **E. Ishow***

1582. Theoretical understanding of thermally activated decay fluorescence property in tetrakis[carbazol-9-yl]benzene derivatives. **P. Peng**, Z. Shuai, Y. Yi

1583. Solution-processed multi photon emission type organic light-emitting devices. **T. Chiba***, Y. Pu, T. Hikichi, S. Ohisa, J. Kido

1584. Improving spectrum purity and brightness of OLEDs based on an open shell radial TTM-1Cz. **A. Obolda**, F. Li

1585. Correlation of charge mobility with energetic disorder of host molecules in *p*-doped organic semiconductors. **S. Yoo**, J. Lee, J. Kim, J. Kim*

1586. Synthesis, characterization, and fabrication of a new series of conjugated light emitting polymers with high color purity and brightness. **P.K. Iyer**, P. Gopikrishna, D. Das

1587. Novel blue naphthalimide derivatives capable of harvesting triplet excitons via triplet fusion, and their applications for efficient white organic light-emitting diodes. **N. Wang**, **Z. Lu**, Y. Huang, F. Li

Hawaii Convention Center
317B

The Frontiers of Geometrically Frustrated Magnetic Materials (#430)

Organized by: C. Wiebe, C. Ling, J. Gardner, H. Zhou

19:00 – 1588. SIKA: A new cold triple axis neutron spectrometer ideal for studies at the frontiers of geometrically frustrated magnetism. **J.S. Gardner***

19:40 – 1589. Multiple-q phases in a stacked triangular antiferromagnetic Heisenberg model with competing interactions under magnetic field. **S. Tanaka***, R. Tamura, K. Tanimoto, K. Totoku

19:55 – 1590. Quantum fluctuations in frustrated organic complexes κ -(ET) $_x$. **Y. Shimizu***, A. Ono, M. Itoh, M. Yoshida, M. Takigawa, M. Maesato, A. Otsuka, H. Yamochi, T. Hiramatsu, Y. Yoshida, G. Saito

20:10 – 1591. Designing mutiferroics with frustrated molecules. **C.D. Batista***

20:25 – 1592. Quantum water ice. **O. Benton**, O. Sikora, N. Shannon

20:40 – 1593. Population of frustrations in the 2D XY model of a finite size square spin ice. **K. Nefedev**

Hawaii Convention Center
319B

Self-assembled Biofunctional Nanomaterials (#433)

Organized by: R. Nagarajan, K. Sakurai, H. Chen

19:00 – 1594. Soft nanotubes for encapsulation, release, and stabilization of proteins. **N. Kamata***, M. Masuda, T. Shinmizu

19:20 – 1595. Impact of packing parameter of synthetic amphiphiles on drug and gene delivery systems. **M.A. Ilies**

19:40 – 1596. Tadpole-shaped polymeric micelle with distinct phase segregation formed from pDNA, block copolymers, and chondroitin sulfate. **K. Osada***, Q. Chen, K.M. Takeda, K. Kataoka

20:00 – 1597. Evaluation of dendritic polymers as transfection agents. **J.A. Kretzmann***, C.W. Evans, D. Ho, B. Garcia-Bloj, P. Blancafort, M. Norret, K. Iyer

20:20 – 1598. Intracellular delivery of fluorescent nanoparticles self-assembled from a cytidic acid-appended fluorescein dye. **R. Iwaura***, K. Yoshida, M. Ohnishi-Kameyama

20:40 – 1599. Preparation of phenylboronic acid-containing frambooidal nanoparticles and their potential application in antioxidant delivery. **M. Morisaki***, A.J. van der Vlies, U. Hiroshi, U. Hasegawa

Friday Morning

Hawaii Convention Center
313C

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi

Presiding: H. Matoussi, G. Sereda

8:00 – 1600. Synergistic DNA delivery with gold-synthetic amphiphile hybrid nano-systems. **M.A. Ilies**

8:15 – 1601. Impact of nanoparticles on the spreading of cell aggregates. **G. Beaune**, F. Brochard-Wyart, F. Winnik*

8:30 – 1602. Silica-containing redox nanoparticles as nanokidney. **Y. Nagasaki***

8:55 – 1603. Self-assembled supramolecular nanosystems for smart targeted therapy of cancer. **K. Kataoka***

9:20 – 1604. Unique properties of double-stranded DNA-functionalized nanoparticles. **M. Maeda***

9:45 Intermission

10:00 – 1605. Multi-coordinating Amphiphilic polymers as a platform for functionalizing metal, metal oxide and semiconductor nanocrystals. **W. Wang**, **H. Matoussi***

10:25 – 1606. Biomolecules on gold nanocrystals: Form and function. **C. Murphy***

10:50 – 1607. Designed chemical synthesis and assembly of uniform-sized nanoparticles for medical applications. **T. Hyeon**

11:15 – 1608. Design of functional nanomaterials by the controlled covalent, coordination, and electrostatic cross-linking. **G. Sereda***, K. Rashwan, J. Keppen, E. Brakke, A. Fritz, S. Schwabbe, G. Bertsch, D. Christianson

11:30 – 1609. Silica-enzyme nanohybrids for biocatalysis. **E. Jackson**, M. Ferrari, D. Cazaban, S. Correa, **L. Betancor***

11:45 – 1610. Stimuli-responsive magnetic nanomicelles as multifunctional heat and cargo delivery vehicles. **E. Rozhkov***, V. Rose, V. Novosad

Hawaii Convention Center
316A

Chemistry and Applications of Graphene (#39)

Organized by: Y. Chen, R. Haddon, K. Loh

Presiding: W. de Heer, J. Huang, D. Li, A.T. Wee

8:00 – 1611. Ballistic nanostructures for epitaxial graphene nanoelectronics. **W. de Heer***

8:20 – 1612. STM/STS studies of graphene nanoribbons and MoS₂ monolayers. **A.T. Wee***, Y. Huang, H. Huang, L. Li

8:40 – 1613. Some new insights about graphene oxide. To burn or not to burn, to dissolve or not to dissolve. **J. Huang***

9:00 – 1614. Graphene as a protective layer for silicon in an aqueous PEC cell. **A.C. Nielander**, N.S. Lewis

9:15 – 1615. Micellar electrokinetic chromatography of graphenes. **T. Takayanagi***, M. Morimoto, Y. Tomiyama, T. Yabutani

9:30 – 1616. Modified graphene oxide for electro-optical switching devices. **M. Kim***, J. Park, G. Scalia, Y. Kim

9:45 Break

10:00 – 1617. Electricity generated by moving water on graphene. **W. Guo**

10:20 – 1618. Multilayered graphene hydrogel membranes. **D. Li**

10:40 – 1619. Local recovery of the electrical conductivity of graphene oxide by vacuum-ultraviolet photoreduction. **Y. Tu***, T. Utsunomiya, T. Ichii, H. Sugimura

10:55 – 1620. Electrical characterization of graphene films synthesized by plasma treatment under a low carbon concentration. **Y. Okigawa**, R. Kato, M. Ishihara, T. Yamada, M. Hasegawa

11:10 – 1621. Influence of the iron oxide nanoparticles on the electronic properties of graphite and few-layers graphene. **M. Quintana***, A. Champi, A. Bazan

11:25 – 1622. Stimuli responsive graphene dispersions and materials. **J. Texter***

Hawaii Convention Center
321A

Nanowires: Synthesis, Fundamental Properties and Novel Device Applications (#51)

Organized by: T. Yanagida, S. Hara, S. Jin, P. Yang, R. Agarwal, L. Lauhon, H. Zheng

Presiding: R. Agarwal, N. Fukata, T. Yanagida

8:00 – 1623. 3D printed bionic nanomaterials. **M. McAlpine**

8:30 – 1624. Nanowire devices for manipulation and analysis of DNA, RNA, proteins, and exosomes. **Y. Baba**

9:00 – 1625. Germanium nanowires-in-graphite tubes via self-catalyzed synergistic confined growth and the Li-storage performance. **C. Wang***, S. Yong*

9:30 Break

9:50 – 1626. Connectivity, memory, and neuromorphic function in nonbiological networks. **J.J. Boland***

10:20 – 1627. Synthesis, characterization, and device fabrication of metal chalcogenides nanostructures for solar and waste-heat energy conversions. **L. Whittaker-Brooks**, A. Rahman

10:30 – 1628. Making graphene nanoribbons: A theoretical exploration. **J. Wang***, L. Ma, F. Ding

10:40 – 1629. Strong diameter dependence of Seebeck coefficient in thin-films of solution-synthesized PbSe and PbTe nanowires. **N. Mishra**, M. Jaime, O. Roslyak, A. Piryatinski, J. Hollingsworth

10:50 – 1630. Perovskite solar cells based on 3D dendritic anatase titania nanowire thin films. **W. Wu**, F. Huang, D. Chen, Y. Cheng, R.A. Caruso*

11:00 – 1631. First-principles simulation on sensing properties of silicon carbide and zinc oxide nanowires. **K. Nakamura***

11:10 – 1632. Thermal and electrical transport in template fabricated poly(3-hexylthiophene)-multiwalled carbon nanotube composite fibers. **M. Smith***, V. Singh, K. Kalaitzidou, B.A. Cola

11:20 – 1633. Columnar liquid crystals in nanochannels of circular and other cross-sections. **R. Zhang**, X. Zeng, Y. Liu, G. Ungar

Hawaii Convention Center
Halls I, II, III

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie

Poster Session

10:00 – 12:00

1634. pH dependence of molecular structures of Dawson-type tri-aluminum-substituted polyoxotungstates. **M. Akawa**, T. Kashiwagi, C.N. Kato*

1635. Hydration of diphenylacetylene catalyzed by phosphanegold(II) cationic species stabilized with polyoxoanion. **H. Arai***, T. Yoshida, K. Nomiya

1636. Enhanced sensitivity of colour-emission switching of fluorescein film by incorporation of polyoxometalate. **L. Bi**

1637. Mode of action of decavanadate in biology. **D.C. Crans***, M. Aureliano

1638. Elucidation of the fast self-assembly of the uranyl peroxide cluster U₃₂-C. Falaise, H. Neal, M. Nyman

1639. Lindqvist polyoxoniobates as aqueous precursors for lithium niobate thin films. **D. Fast**, Y. Hou, L.B. Fullmer, S.R. Decker, M. Nyman, M. Dolgos

1640. Polyoxometalates to metal oxide thin film: the effect of protonation. **L.B. Fullmer**, R.H. Mansergi, L.N. Zakharov, D.A. Kesler, M. Nyman

1641. Rare earth(III) salts diphosphato- and diphenylphosphonato-tetraperoxido-hept tungstates. **D. Shima***, M. Hashimoto

1642. Assembly of photoactive organic polyoxometalate complexes. **M.R. Healey**, K.M. Davies, C. Ritchie*

1643. Keggin-type platinum(II)-coordinated polyoxotungstates: Syntheses, molecular structures, and photocatalytic performance for hydrogen evolution from water under visible light irradiation. **Y. Ihara**, S. Hattori, K. Aono, R. Yamashita, C.N. Kato*

1644. Molecular chirality and racemization behavior of sandwich-type polyoxometalolanthanates. **J. Iijima***, H. Naruke

1645. Reversible structural conversion of chloride-incorporated dodecavanadates for release control of the chloride. **Y. Inoue**, Y. Kikukawa, Y. Hayashi*

* Principle Author

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onlineprogram

- 1646.** Open-Dawson polyoxometalates containing tetraaluminum, tetr gallium, and decaindium hydroxide clusters. **Y. Inoue**, S. Matsunaga, O. Takyua, K. Nomiya
- 1647.** Visible-light-responsive multielectron redox catalysis utilizing electron transfer from coordinated alcohols to lacunary polyoxometalates. **J. Jeong**, K. Suzuki, K. Yamaguchi, N. Mizuno*
- 1648.** Evaluation of a structural ion fluctuation in Preyssler-type polyoxometalate salt. **C. Kato**, S. Nishihara, K. Maryunina, R. Tsunashima, Y. Tatewaki, K. Inoue
- 1649.** Syntheses, molecular structures, and acid catalysis of organozirconium complexes with Keggin-type mono-aluminnum-substituted polyoxotungstates. **S. Kato**, T. Ogasawara, C.N. Kato*
- 1650.** Mesoporous ionic crystals constructed with cationic metal complexes ($M = Cr^{3+}, Fe^{3+}$) and anionic polyoxometalates: Importance of water clusters as templates. **R. Kawahara**, K. Niinomi, S. Uchida*
- 1651.** Control of composition and structure in decavanadate-alkylamine hybrid layered crystals. **Y. Kiyota**, T. Kojima, H. Naruke, M. Kawano, T. Ito
- 1652.** Syntheses of inorganic-organic hybrid crystals composed of octamolybdates and heterocyclic surfactants. **J. Kobayashi**, E. Ishikawa, H. Naruke, S. Koguchi, T. Ito
- 1653.** Paddle-polyoxometalates as oxidation co-catalysts in photocatalytic H_2 evolution. **F. Li***, M. Liu, L. Xu
- 1654.** New organic-inorganic hybrid based on dimeric $[Mn_2V_{22}O_6]^{10-}$ polyoxoanion. **Y. Lu***, D. Liu, E. Wang
- 1655.** Driving polyoxometalates to dense thin films: TMA^+ vs. H^+ . **R.H. Mansergh**, L.B. Fullmer, D. PARK, M. Nyman, D.A. Keszler
- 1656.** Construction of manganese and cobalt cores stabilized in polyoxovanadate ligands. **T. Maruyama**, Y. Kikukawa, Y. Hayashi*
- 1657.** Open-Dawson polyoxometalate containing mixed-valence trimanganese cluster. **S. Matsunaga**, Y. Inoue, K. Nomiya*
- 1658.** Inorganic anionic cage $[{\alpha-Si_2W_{18}O_{62}}]^{8-}$ with reversible proton capturing inside the aperture via intramolecular hydrogen bonds. **T. Minato**, K. Suzuki, K. Kamata, N. Mizuno*
- 1659.** Synthesis of heterogeneous catalyst composed of aluminum hydroxide cluster polycation and $[SiV_3W_9O_{40}]^{7-}$. **K. Mizuno**, S. Uchida*
- 1660.** Controlled assembly of polyniobate chains in solution monitored by SAXS. **P.I. Molina**, J. Son, W.H. Casey, M. Nyman*
- 1661.** Synthesis of heterogeneous catalysts composed of aluminum hydroxide cluster and $[CoW_{12}O_{40}]^{6-}$. **T. Murai**, S. Uchida*
- 1662.** Mo_4^{2-} ($M = Mo, W$) encapsulating silver(I) ethynide clusters formed by template exchange reactions abstracting Mo_4^{2-} groups from the Keggin-type polyoxometalates. **K. Ohashi**, T. Kojima, T. Ozeki*
- 1663.** Novel phosphonium and ammonium hexatungstate compounds for the precursor of inorganic photoresists: Synthesis and radiation chemistry. **S. Saha***, J.M. Amador, S.R. Decker, L.N. Zakharov, D.A. Keszler*
- 1664.** Construction of chiral polyoxometalate/nanoparticle composites toward chirality transfer and enhancement. **L. Shi**, L. Wu*
- 1665.** Synthesis and structure of di- and triphosphato complexes of peroxovanadate. **S. Sorihashi**, M. Hashimoto
- 1666.** Modification of zirconium-substituted polyoxometalates for peroxidase-like catalysis. **Y. Wang***, H. Tan
- 1667.** Liquid-crystalline materials with an inorganic core in mesogen. **R. Watanabe**, T. Tsurumi, S. Yamada, O. Tsutsumi*
- 1668.** Thermodynamic stability of aqueous metal clusters: A dynamic approach. **L. Wills**, T. Mustard, I. Chang, P.H. Cheong
- 1669.** Synthesis of novel photochromic polyoxometalate compounds. **J. Xu**, M.R. Healey, C. Ritchie
- 1670.** Base catalysis of niobate clusters. **S. Yamazoe**, S. Hayashi, K. Koyasu, T. Tsukuda*
- 1671.** Assembly of coordination-adjustable units to form inorganic-organic hybridized molecular-scale proton conductors. **H. Zang***
- 1672.** Synthesis and characterization of Sb-bisected heteropolyoxoniobate microtubule. **Z. Zhang***, J. Peng*, W. Zhou*
- 1673.** Like-titanium-oxo-clusters with salicylic and phthalic ligands. **Q. Zhu***, J. Dai*, J. Hou
- Hawaii Convention Center
318A
- Two-dimensional Nanosheets and Nanosheet-Based Materials: Synthesis, Characterization, Functionalization and Applications (#95)**
- Organized by: J. Kawamoto, J. Choy, C. Detellier, H. Zhang, J. Huang, L. Wan
Presiding: C. Detellier, H. Usami
- 8:00 – 1674.** From 2D nanosheet to 3D multifunctional nanohybrids. **S. Hwang**
- 8:30 – 1675.** Macrosopic hierarchical structures of liquid crystalline inorganic nanosheets. **T. Nakato***, Y. Nono, E. Moura
- 8:50 – 1676.** Cellulose nanomaterials by unconventional ball milling. m. Zhao, **S. Kuga**, M. Wu*, Y. Huang
- 9:10 – 1677.** Chromium halide nanosheets – 2D insulating ferromagnets for spintronic application. **D. Weber**, L.M. Schoop, A. Kuhn, B.V. Lotsch*
- 9:30 – 1678.** Bandgap-tunable lateral and vertical heterostructures based on monolayer $Mo_{1-x}W_xS_2$ alloys. **Y. Kobayashi**, S. Mori, Y. Maniwa, **Y. Miyata***
- 9:50 Break**
- 10:00 – 1679.** Host-guest chemistry of nanospace materials. **M. Ogawa**
- 10:30 – 1680.** Solvation induced excimer formation in clay-fluorescent dye hybrid systems. **Y. Suzuki***, M. Tominaga, Y. Oniki, J. Kawamoto
- 10:50 – 1681.** Excitonic and photoluminescent properties of laterally confined 2D transition-metal dichalcogenides. **B.J. Carey**
- 11:10 – 1682.** Anisotropic photothermal response of the poly(*N*-isopropylacrylamide) gel hybridized with liquid crystalline clay nanosheets aligned by electric field. **N. Miyamoto***, T. Inadomi
- 11:30 – 1683.** Particle size and surface charge effect of layered double hydroxide nanoparticles in their surface interaction with biological substances. **J. OH***, H. Kim, I. Hong, T. Kim
- 11:55 Closing Remark**
- Hawaii Convention Center
Halls I, II, III
- Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101)**
- Organized by: F. Vetrone, S. Kohei, D. Ma, W. Huang, L. Huang, X. Peng
- Poster Session**
- 10:00 – 12:00**
- 1684.** Unconventional white-light emission of CdSe core quantum dots synthesized at room temperature. **N. NAGASHIMA**, K. KONDOH, T. UWADA, **M. Ishikawa***
- 1685.** Fabrication and characterization of a silver mirror planar microcavity with organic dye J-aggregates. **H. Mizuno***, N. Tanigiri, Y. Kawanishi, A. Ishizumi, H. Yanagi, I. Hiromitsu
- 1686.** Monochromatic and white light LEDs from carbon nanoparticles. **W. Yu***
- 1687.** Multicolor upconversion luminescence by adding Er^{3+} in β -NaYF₄:Yb³⁺/Tm³⁺ phosphor. **H. Lin**, D. Xu, D. Teng, S. Yang, Y. Zhang*
- 1688.** Fluorescence properties of peryleneimide nanoparticles prepared by reprecipitation method. **S. SASAKI***, T. Asahi
- 1689.** Fabrication of ZnS-AgInS₂ nanoparticles covering on SiO₂ particles and characterization of their fluorescence property. **Y. Saito**, Y. IMURA, H. Endo, T. Kawai
- 1690.** Glucose-powered antimicrobial system using organic-inorganic assembled network materials. **I. Iiu**
- 1691.** Multiple ZnS coating method for high-efficiency Cd-free quantum dot. **T. Fukuda***, T. Kurabayashi, M. Hishinuma
- 1692.** Sol-gel preparation and luminescence properties of Mn²⁺-doped Zn₂GeO₄ and Li₂ZnGeO₄ thin film phosphors. **M. Karita**, T. Sanada, N. Wada, K. Kojima
- 1693.** Preparation of Tb³⁺-doped Ta₂O₅ fluorescent, spherical particles by sol-gel method using W/O emulsion and their characterization. **S. Oku**, T. Sanada, N. Wada, K. Kojima
- 1694.** Highly efficient upconversion in Zn₂TiO₄: [Er, Yb] phosphor for biomedical application. **S. Yamamoto**
- 1695.** Organic fluorescent nanoparticles encapsulating a liquid pyrene. **S. Azeyanagi**, K. Hayashi, M. Taki, Y. Sato, T. Higashiyama, S. Yamaguchi*
- 1696.** Preparation of highly photoluminescent, low cytotoxic small glass particles incorporating quantum dots. **M. Ando***
- 1697.** Synthesis of blue-light emitting alkyl-passivated silicon nanocrystals via $(HSiO_3)_n$ sol-gel polymer. **Y. Xin**, R. Wakimoto, D. Kajya, K. Saitow*
- 1698.** Rational design of a conjugated molecule based on donor-acceptor (D-A) structure as the fluorescent probe to picric acid. **H. Ma***, C. He, F. Li, M. Zhang
- 1699.** Y³⁺ doping effect on phase and size of LiGdF₄-based upconversion nanoparticles. **H. Na**, J. Jeong, H. Chang, H. Kim, K. Mkohyan, **H. Jang**
- 1700.** Increasing efficiency of small molecular/polymer hybrid organic semiconducting thin films for light emitting diodes. **H. Kon**, C. Kurosova, Y. Tsuji*
- 1701.** Nonconjugated poly(maleimide-alt-methacrylate): Unusual luminescence and ion-sensing properties. **J. Yan**, D. Pan, R. Yang, Y. Xu, L. Wang, M. Yang
- 1702.** Estimation of defect density in oxyantride and nitride photocatalysts by fluorescence lifetime measurement. **N. Koshimizu**, C. Izawa, T. Watanabe
- 1703.** High luminescent size-tunable silicon quantum dots and their applications for sensing explosives. **B. Cho**, H. Sohn*
- 1704.** Synthesis and properties of K_2TiF_6 : Mn²⁺ phosphors by continuous coprecipitation method. **C. Kim***, S. Jee, B. Bang, K. Choi
- 1705.** Fabrication of Sr₂MgSi₂O₇ (SMS): Eu²⁺ phosphors by the solid-state reaction and sol-gel process. **A. Matsunaga***, T. Nishiki, R. Asano, T. Kido, K. Matsui
- 1706.** Proton-responsive emission properties in cyclometalated iridium(III) complex film, $[Ir^{III}(bpd)]_n$ Na⁺ (bpd = 2,4'-(benzene-1,3-diyl)dipyridine). **H. Kamebuchi***, Y. Fujimura, A. Okazawa, M. Tadokoro, N. Kojima
- Hawaii Convention Center
320 Theatre
- Functional Molecular Materials and Devices (#128)**
- Organized by: R. Kato, H. Mori, J. Schlueter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya
Presiding: R. Kato, T. Mori
- 8:00 Introductory Remarks**
- 8:05 – 1707.** Switching of organic superconductivity by electric-field, strain, and light. **H.M. Yamamoto***
- 8:30 – 1708.** Naphtho[2,3-*b*:6,7-*b'*]dithiophene-4,5,9,10-diene (NDT)-based organic semiconductors: From small molecules to polymers. **K. Takimiya**, M. Nakano, J. Hu, I. Osaka
- 8:55 – 1709.** N-shaped pi-conjugated materials with high carrier mobility and thermally stable crystal phase in solution crystallized organic field-effect transistor. **C. Mitsui**, M. Yamagishi, K. Yoshimoto, J. Soeda, H. SATO, A. Yamano, J. Takeya, T. Okamoto
- 9:15 – 1710.** Phosphorescent metal complexes for organic light-emitting application. **S. Lo***, R. Wawrzinek, M. Ullah, K. Muhieddine, P. Koszo, P.E. Shaw, P.L. Burn, E. Namdas*
- 9:35 – 1711.** Formation of the conductive interface by conjugating electron donor and acceptor single crystals. **Y. Takahashi**, T. Shimada, H. Hasegawa, J. Harada, T. Inabe
- 9:55 break**
- 10:10 – 1712.** Chiral conductors based on methylated TTF derivatives. **N. Avaravi***
- 10:35 – 1713.** When halogen bonding interactions influence the electronic properties of molecular conductors. **M. Fourmigue***, K. Shin, O. Jeannin, J. Lieffrig
- 11:00 – 1714.** Hydrogen-bonded purely organic conductors based on catechol-TTF: Hydrogen-bond-dynamics-based switching of conductivity and magnetism. **A. Ueda***, S. Yamada, T. ISONO, A. Hatakeyama, A. Nakao, R. Kumai, H. Nakao, Y. Murakami, K. Yamamoto, Y. Nishio, H. Mori
- 11:20 – 1715.** Structural and physical properties of molecular conductors derived from chiral and racemic π -donors. **J. Yamada***, S. Inagaki, S. Sakamoto, T. Kadoya, H. Akutsu
- 11:40 – 1716.** Molecular conductors based on TMTTP and its related donors. **Y. Misaki***, T. Shirahata, S. Kohno, Y. Harada, K. Furuta, T. Kawamoto, T. Mori
- Hawaii Convention Center
321B
- Applications of Ultrasound to Nanoscience (#150)**
- Organized by: K. Suslick, F. Grieser, M. Atobe, J. Yu, S. Jeong
Presiding: K. Suslick
- 8:00 – 1717.** Ultrasonic fabrication of composite material. **M. Ashokkumar**
- 8:30 – 1718.** Innovative ultrasonic technology for production of antibacterial nanoparticles and antibacterial textiles. **A.V. Abramova**, **V.O. Abramov***, V.M. Bayazitov, A. Sidorenko
- 8:50 – 1719.** Ultrasonic preparation of gold nanoparticles from bulk gold source. **D. Huber**, J. Watt, M. Austin
- 9:10 – 1720.** Ultrasound assisted synthesis of nanocomposites for energy and environmental remediation. **N. Bernaudoshaw***
- 9:40 – 1721.** Sonochemical preparation of nanocarbon supported Pt catalysts for fuel cells. **S. Hatana***
- 10:10 Coffee and Bio Break**
- 10:20 – 1722.** Application of ultrasound for crystallization and nanoparticle deposition onto surfaces. **J. Lee**, N. Perkas, M. Ashokkumar, A. Gedanken
- 10:50 – 1723.** Fabrication of some mesoporous semiconductors through ultrasonic irradiation at room temperature. **c. yu***, J. Li, J. Yu
- 11:20 – 1724.** Sonochemical synthesis of 2D nanosheets/noble metal nanocomposites for electrochemical applications. **J. Zhu**

* Principle Author

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Hawaii Convention Center
322AB

Janus Materials: Design, Fabrication and Properties (#210)

Organized by: Z. Yang, S. Granick,
E. Kumacheva
Presiding: Z. Yang

8:00 opening

8:05 – 1725. Janus particles for probing and manipulating immune functions. **Y. Yu**
8:35 – 1726. Polymer single crystal templated Janus hybrid hairy nanoparticles. **C. Li**

9:05 – 1727. Dynamically interacting and self-reconfiguring assemblies of Janus microcubes: New actuation principles for microbots and colloidal origami. **K. Han, C. Shields, G.P. Lopez, B. Bharti, O.D. Velev***

9:35 break

9:50 – 1728. Design and fabrication of Janus particles from spherical polymeric templates with the assistance of carbon dioxide. **Q. Yang*, K. Loos***

10:10 – 1729. Proving the Janus character of gold nanoparticles by means of infrared reflection absorption spectroscopy (IR-RAS). **S.D. Bourone*, C. Kaulen, U. Simon**

10:30 – 1730. Microfluidic-assisted synthesis of Janus polymeric microcarriers for dual drug sustained release. **I.U. Khan, C.A. Serra, N. Anton, T. Vandamme, I. Kraus, Z. Chang**

10:50 – 1731. Induced assembly of asymmetrically-functionalized gold nanoparticles using localized DNA hybridization. **L. Pruden, R. Goldstein, A. Liu, E. Hulkko, B. Mayukh, V.A. Apkarian, J.S. Shumaker-Parry**

11:10 – 1732. Janus nanomaterials for thermoelectrics: Manipulating the structure of sulfur based chalcogenides to enhance energy conversion efficiency. **D. Mott*, M.S. Singh, K. Gupta, M. Koyano, S. Maenosono**

11:30 – 1733. Computer simulation of self-assembly for soft Janus particles. **Z. Sun***

Hawaii Convention Center
315

Carbon Nanotubes: Preparation, Characterization and Applications (#227)

Organized by: S. Maruyama,
R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: J. Liu, S. Maruyama

8:00 – 1734. State-of-the-art science and applications of carbon nanotubes. **M. Endo*, H. Muramatsu, K. Takeuchi, T. Hayashi**

8:30 – 1735. How we can realize chirality-specific growth of single-walled carbon nanotubes using intermetallic compound nanocatalysts. **Y. Li**

9:00 – 1736. Toward selective synthesis and applications of carbon nanotubes. **A.R. Harutyunyan**

9:30 – 1737. Quantum chemical simulations of SWCNT and graphene nucleation with and without catalysts. **A. Page**

9:50 break

10:10 – 1738. Perfect ultralong carbon nanotube and its application. **F. Wei***

10:40 – 1739. Sweet spot in the synthesis of single wall carbon nanotube forests and its relation to their properties. **D.N. Futaba**

11:10 – 1740. Modulating diameter of single-walled carbon nanotubes in alcohol catalytic chemical vapor deposition. **R. Xiang, K. Cui, A. Kumamoto, H. An, T. Inoue, S. Chiashi, Y. Ikuhara, S. Maruyama**

11:30 – 1741. Controllable growth of semiconducting and metallic SWCNTs. **P. Hou, C. Liu, H. Cheng***

Hawaii Convention Center
Halls I, II, III

Advances in Bioinspired and Biomedical Materials (#245)

Organized by: K. Healy, Y. Ito,
P. Messersmith, X. Chen, I. Kang
Presiding: P. Messersmith

Poster Session

10:00 – 12:00

1742. Engineered nanostructures of lipopolysaccharide for investigation and regulation of the activation of dendritic cells. **Y. Liu*, K. Wang, M. Zhang, H. Chen, J. Li, S. Ross, F. Liu, G. Liu***

1743. Development of injectable chelate-setting β -tricalcium phosphate cement with non-fragmentation property and their material characteristics. **K. Nagata, M. Honda, T. Konishi, M. Aizawa***

1744. Developmental responses of hippocampal neurons on various functionalized surfaces. **M. Kim*, H. Moon, M. Park, J. Park, I. Choi***

1745. Poisson ratio of collagen fibrils under tension. **H. Wells*, K.H. Sizeland, H. Kayed, N. Kirby, A. Hawley, S. Mudie, R.G. Haverkamp**

1746. Preparation of hydroxyapatite-coated PS plates and culture of human mesenchymal stem cell. **R. Suzuki, K. Iijima, N. Kiyokawa, M. Hashizume**

1747. Morphology control of polysaccharide composite hollow fibers using microfluidic techniques. **S. Ohyama, K. Iijima, K. Yuyama, M. Hashizume***

1748. Effect of carbonated apatite on osteoclast differentiation of RAW264. **Y. Kuwamura*, N. Horiochi, K. Hashimoto, K. Yamashita, A. Nagai**

1749. Evaluation of proliferation of fibroblasts on chondroitin sulfate/chitosan composite films prepared by hot press techniques. **Y. Tsuji, K. Iijima, A. Kakimoto, R. Ninomiya, T. Iyoda, F. Fukai, M. Hashizume**

1750. All-conductive-polymer Interface to electrically guide neurite outgrowth. **Q. Pan, Y. Zhang, B. Zhu***

1751. Mineralization of hydroxyapatite onto crosslinked water-based chitosan/chitin whisker composite nanofibrous scaffold. **A. Pang***

1752. Development of heparin-modified silk fibroin for tissue engineered cardiac patch. **R. Kubo*, K. Shimada, R. Tanaka, Y. Nakazawa**

1753. Improvement of cellular compatibility on titanium surface through a low power laser irradiation in air. **T. Kozuka*, M. Yamane, N. Ohtsu**

1754. Highly ordered 1D fullerene crystals for concurrent control of macroscopic cellular orientation and differentiation towards large-scale tissue engineering. **K. Minami*, Y. Kasuya, T. YAMAZAKI, Q. Ji, W. Nakaniishi, J. Hill, H. Sakai, K. Ariga***

1755. Bioinspired coating of tissue engineering scaffolds in regenerative medicine. **H. Shin*, J. Lee, S. Madhurakkat Perikama**

1756. Development of a seeded scaffold in the great omentum feasibility of an *in vivo* bioreactor for esophageal reconstruction. **E. Chung*, C. Park**

1757. Characterization of silk fibroin/poly(ethylene carbonate) composite films for cardiac patches. **A. Yonezawa, Y. Nakazawa, Y. TOMINAGA**

1758. Novel chelate-setting cements with various calcium-phosphate phases for minimally-invasive treatment of bone disease: Processing, material property, in vitro solubility, and biocompatibility. **K. Hazama, K. Nagata, M. Honda, M. Aizawa***

1759. Structure and strength of neonatal pericardium for heart valve application. **K. Sizeland*, H. Wells, J. Higgins, C. Cunanan, N. Kirby, A. Hawley, S. Mudie, R.G. Haverkamp**

1760. Effect of the addition of the vanadium ion in the property of β -tricalcium phosphate ceramics. **Y. Sekiguchi***

1761. Development of silk fibroin/polyurethane composite materials for degradable cardiac patch. **A. Higuchi, R. Kubo, A. Asano, C.T. Nakazawa, R. Tanaka, K. Shimada, T. Kameda, Y. Nakazawa**

1762. Modification of gelatin nanofiber with genetically engineered growth factor. **K. Toyonaga*, Y. Mashimo, M. Mie, E. Kobatake**

1763. Fabrication of β -tricalcium phosphate ceramics substituted with silicon. **K. Hashimoto*, H. Shibata**

1764. Preparation of a sintered body of β -Ca₂SiO₄/ β -NaCaPO₄ solid solution as new bioceramics. **I. WATANABE*, H. Shibata, K. Hashimoto**

1765. Tailoring micrometer-long high-integrity 1D array of superparamagnetic nanoparticles in a nanotubular protein jacket and its lateral magnetic assembling behavior. **S. Sim*, D. Miyajima, T. Aida**

1766. Initiation of enzyme-catalyzed polymerization by the chemical structural transformation of the substrates. **T. Waga, Y. KIKKAWA, K. Hiratani, H. Endo, T. Kawai**

1767. Development of RGD containing hydrophobic extracellular matrix for small-caliber vascular grafts. **N. Nishioka*, Y. Mashimo, M. Mie, E. Kobatake**

1768. High speed water transport on open channels controlled by arrangement of structures. **K. Muto, S. Ito, D. Ishii**

1769. Expression and purification of a functional silica binding protein fused with RGD motif for neural tissue engineering. **M. Yang*, W. Chen, A. Masroujeh, A. Augustine, C. Tsai, Y. Chen-Yang***

1770. Novel chemoembolization on the basis of porous calcium-phosphate microspheres prepared by salt-assisted ultrasonic spray-pyrolysis technique. **M. Aizawa*, S. Yabu, K. Yano, M. Matsueda, M. Honda, M. Emoto**

1771. Design and synthesis of artificial TRAIL mimics based on C₃-symmetric and luminescent iridium complexes. **A.A. Masum, H. Tanaka, N. Suzuki, Y. Hisamatsu, S. Aoki**

1772. Antimicrobial peptide stars: The road to discovery and development. **S. Lam, N. O'Brien-Simpson, N. Pantarat, A. Sulistio, E. Wong, A. Blencowe, E. Reynolds, G.Q. Qiao***

1773. Mussel-inspired, facile antibacterial coatings onto various substrates. **D. Kim, J. Moon, S. Song, J. Choi*, W. Cho***

1774. Cell-instructive bioactive hydrogel with microchanneled piezoelectric membrane. **S. Cho, M. Lee, H. Kong, J. Jeong***

1775. Cellular responses of osteoblasts to nitrogen-doped hydroxyapatite ceramics: Cell attachment, proliferation, morphology, differentiation, and calcification. **R. Namiki, R. Umeda, R. Hashimoto, C. Izawa, M. Nakamura, M. Honda, T. Watanabe, M. Aizawa***

1776. Cellular evaluation of beat-tricalcium phosphate doped with potassium or sodium. **A. Muto*, H. Shibata, K. Hashimoto**

1777. Worm-inspired microneedle patches for enhanced adhesion and controlled release of drugs. **K. Seong, Y. Hwang, S. Yang***

1778. Fabrication of vascular endothelial growth factor-loaded apatite-fiber scaffolds with enhanced mechanical property and their biological evaluation. **S. Yasuda, M. Honda, M. Nagaya, Y. Asano, K. Nakano, H. Nagashima, M. Aizawa***

1779. Development of angiogenic peptides /silk fibroin sheet for coronary vascularization. **K. Takahama, K. Shimada, R. Shimada, A. Yonezawa, R. Tanaka, S. Nemoto, Y. TOMINAGA, T. Kameda, Y. Nakazawa**

1780. Clarification of interaction of denatured protein on artificial dialysis membrane. **Y. Chikayama*, Y. Ueno, H. Takahashi, M. Yamada, F. Fujieda, K. Hayashi, H. Nakamura**

1781. Novel Al-rich microtubular sheaths produced by an Fe-oxidizing bacterium, *Leptothrix*, in culture. **K. Tamura, T. Kunoh, H. Kunoh, J. Takada***

1782. Mussel-inspired, self-healing polyurethane elastomers blended with poly(dopamine methacrylate). **S. Song*, Y. Tang*, X. Qu*, Z. Yang*, J. Huang***

1783. Dopamine as a new tanning molecule for mandible development in grasshoppers. **K. Lee, H. Lee***

1784. New molecule in self-assembled monolayer for super-hemophilic modification of platinum surfaces. **H. Lee, I. Song, H. Lee***

1785. Repairable and stimuli-responsive cathecolamine film inspired by insect cuticular melanization. **Y. Wang, H. Lee***

1786. Theoretical study of the interaction of aminoglycosides and gold complexes with different sequences of HIV ARN molecules. **P. Francisco Santiago*, B. Molina Brito, J. Soto Mercado, L. Sansores Cuevas**

1787. Construction of bFGF-tethered ECM for tissue engineering. **C. Sutinont*, Y. Mashimo, M. Mie, E. Kobatake**

1788. Antibacterial behaviors of Ag-contained apatite coating on titanium substrate fabricated using calcium-phosphate slurry. **Y. Kakuchi*, M. Hirano, M. Komata, N. Ohtsu**

1789. Antimicrobial and antibiofilm activities of cellobiose dehydrogenase functionalized polydimethylsiloxane. B. Thallinger*, M. Brandauer, K. Gitschalter, C. Sygmund, R. Ludwig, G.S. Nyangongo, G.M. Guebitz

1790. Intracellular acidity-responsive polymer-drug conjugates for malignancy therapy. **X. Zhuang*, J. Ding, X. Chen**

1791. Construction of a molecular logic gate inspired by polymerase chain reaction. **T. NOJIMA***

Hawaii Convention Center
319A

Self-organization of Membrane Systems (#259)

Organized by: D. Sasaki, K. Morigaki, I. Koepfer
Presiding: D. Sasaki

8:00 – 1792. Applications of artificial lipid-anchored proteins to study membrane protein behavior in vivo and in vitro. **J.R. Silvius***

8:30 – 1793. Membrane deformation determined by intracellular viscosity. **K. Fujiwara, M. Yanagisawa**

8:50 – 1794. Role of protein crowding in shaping and organizing cellular membranes. **J. Stachowiak***

9:20 – 1795. Enhanced order of lipid bilayer by n-alkane. **M. Hishida*, A. Endo, R. Yanagisawa, K. Nakazawa, Y. Yamamura, K. Saito**

9:40 – 1796. Controlling membrane dynamics by tuning the hydrophobic mismatch. **M. Nagao*, E.G. Kelley, R. Ashkar, R.D. Bradbury, K. Wood, A.C. Woodka, X. Zuo, P.D. Butler**

10:00 – 1797. Applications of model membrane architectures. **S.G. Boxer***

10:30 – 1798. The phage endolysin PlyC penetrates bilayer membranes after docking to phosphatidylserine. **M. Barros, F. Heinrich, T. Vennemann, M. Lüsche*, D. Nelson**

* Principle Author

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<http://pacifichem.org/onlineprogram>

10:50 – 1799. Magnetically directed 2D crystallization of membrane proteins in block copolymers. S. Klara, P. Saboe, I. Sines, M. Kumar, **M.S. Mauter**

11:10 – 1800. Osmotic stress induced stochasticity in *E.coli* synthetic gene network. **S. Muralidharan***, G. Balandaram, S. Srividya, A. Peasley

11:40 – 1801. Chiral recognition of L-amino acid on liposome prepared by L-phospholipid. T. Ishigami, K. Suga, Y. Okamoto, **H. Umakoshi***

Hawaii Convention Center
318B

Advanced Materials for Photonics and Electronics: Fundamentals and Applications (#308)

Organized by: R. Morandotti, D. Moss, F. Omenetto, N. Tsutsumi, K. Alamgir, K. Char, A. Facchetti
Presiding: R. Morandotti

8:00 – 1802. Highly aligned lamellar block copolymer films for high energy-density electrostatic capacitors. S. Samant, C. Grabowski, K. Kisslinger, M. Durstock, **A. Karim***

8:30 – 1803. Decipher supramolecular nanocomposite toward functional material. **T. Xu**

9:00 – 1804. Neutron crystal structure analysis of stilbazolium derivatives for developing nonlinear optical materials with low terahertz-wave absorption. **T. Matsukawa***, Y. Yoshida, A. Hoshikawa, S. Okada, T. Ishigaki

9:20 – 1805. Selective noncontact modification of morphology and chain orientation in conducting polymers by femtosecond laser writing. **H. Lee**, S. Chae, S. Lee, J. Choi, H. Kim

9:40 – 1806. OBDD-forming block copolymer for a photonic crystal: Effect of particle distortion on SAXS studied by paracrystalline theory and self-consistent field theory. **S. Okamoto***, K. Nomura

10:00 break

10:10 – 1807. Observation of significantly increased Rayleigh scatter in UV-exposed optical fiber and its application in distributed sensing. S. Loranger, M. Gagne, V. Lambin lezzi, **R. KASHYAP**

10:40 – 1808. Development of high-refractive index titanate-silk nanocomposites for biopolymer-based optical devices. G. Perotto, F. Omenetto, **A. Martucci**

11:00 – 1809. Theoretical study of 3D nano optical assembling. **T. Iida***, M. Tamura

11:20 – 1810. Investigation of grating-coupled SPR enhanced organic photovoltaic cells fabricated by pressure-less nanoimprinting technique. **S. Nootchanat***, A. Pangdam, R. Ishikawa, C. Thammachareen, K. Shinbo, K. Kato, F. Kaneko, N. Tsuboi, S. Ekgasit, A. Baba*

11:40 – 1811. Understanding the effect of hydrogen passivation of impurities in solution processed metal oxide thin film. **J.C. Ramos**, L. Feixiang, C. Perkins, D. Park, Y. Huang, E. Garfunkel, D.A. Kesler

Hawaii Convention Center
319B

Membranes and Nanotechnologies for Energy and Environment Applications (#317)

Organized by: H. Park, B. Freeman, B. McCloskey, J. McGrath, A. Hill, A. Higuchi, Y. Lee

8:00 – 1812. High free volume polymer membranes for gas separation. **P.M. Budd***

8:30 – 1813. Role of adaptive porous frameworks in anti-aging mixed matrix membranes. **C. Lau***, S. Smith, K. Konstas, A. Thornton, A.J. Hill, M.R. Hill

8:50 – 1814. Microporous polyimides incorporating Tröger's Base for membrane gas separation. **M.D. Guiver**, Y. Zhuang, J. Seong, Y. Do*, H. Jo, Y. Lee

9:10 – 1815. Ladder-structured polysilsesquioxane-based hybrid membranes for gas separations. **J. Lee***, S. Park, A. Lee, S. Hwang

9:30 – 1816. High-performance triptycene-based gas separation membranes. **I. Plnau***, B. Ghanem, R. Swaidan, E. Litwiler

9:50 – 1817. New membranes and membrane unit operations for a process intensification strategy. **E. Drioli**, F. Macedonio

10:20 – 1818. Advanced polymeric membrane for gas separation. **K. Nagai***

10:40 – 1819. Surface modification of nanoporous polysulfone ionomers for VRFB applications. **B. Gindt**, Z. Tang, D.G. Abebe, T. Zawodzinski, T. Fujiwara*

11:00 – 1820. Recent developments to describe and predict gas solubility and permeability in glassy polymeric membranes. **G.C. Sarti***

11:20 – 1821. Architecturing molecular cavities in ptycene-containing polyimide membranes for gas separation. **R. Guo***, S. Luo, J. Wiegand, Q. Zhang, G. Kline

11:40 – 1822. New use for MOFs: Stopping physical aging in glassy polymers for exceptional separation performance. **M.R. Hill***, C. Lau, A.J. Hill, K. Konstas, R.D. Noble, C.M. Doherty, D. Gin, T.J. Bastow

Hawaii Convention Center
316C

Ceramic Materials and Processing for Advanced Applications (#341)

Organized by: F. Rosei, A. Vomiero, Y. Tachibana, C. Raston, H. Zhang

8:00 – 1823. Interfacial nanoengineering of perovskite solar cells based on $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{HC}(\text{NH}_2)_2\text{PbI}_3$. **N. Park**

8:30 – 1824. Charge separation and recombination dynamics at $\text{TiO}_2/\text{Perovskite}/\text{OMeTAD}$ interfaces. M. Liu, S. Makuta, M. Endo, A. Wakamiya, **Y. Tachibana***

8:50 – 1825. Toward efficient perovskite solar cells: Development of new charge-transporting materials and surface treatment of lead halide perovskite layer. **A. Wakamiya***, H. Nishimura, N. Maruyama, A. Shimazaki, N. Nakaike, M. Endo, T. Aihara, Y. Murata

9:10 – 1826. Panchromatic dye-sensitized solar cells for spectral splitting photovoltaics using lead halide perovskite solar cells. **T. Kinoshita***, S. Uchida, H. Segawa

9:30 coffee break

9:50 – 1827. Organic lead halide perovskite for high efficiency solar cells and optoelectronic devices. **T. Miyasaka***

10:20 – 1828. Electronic and energetic landscape of perovskite solar cell: A microwave conductivity study. **A. Saeki**

10:40 – 1829. Investigation of surface treatment for stable and efficient planar heterojunction perovskite solar cells. **L. Cojocaru***, S. Uchida, J. Nakazaki, T. Kubo, H. Segawa

11:00 – 1830. Planar heterojunction perovskite solar cells using sequential vacuum deposition method for high stability and low-cost. **K. Yamamoto**, M. Shahiduzzaman, Y. Furumoto, T. Kuwabara, K. Takahashi, T. Taima*

11:20 – 1831. Controlling charge recombination dynamics by modifying conjugated polymer/ ZnO nanocrystal interface for hybrid solar cell applications. M. Liu,

Y. Tachibana*, W. Li, M. Purushothaman, Z. Ma, J.S. Chen, S.K. Matta

11:40 – 1832. PbS quantum-dot/ ZnO nanowire solar cells yielding high efficiency in the near-infrared region and long-term stability. **H. Wang***, T. Kubo, J. Nakazaki, H. Segawa

Hawaii Convention Center
317B

Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei, A. Wee, W. Chen, P. Weiss
Presiding: D. Perepichka

8:00 Introductory Remarks

8:05 – 1833. Molecular Self-Assembly on graphene and graphite: From fundamentals to applications. **S. De Feyter***

8:35 – 1834. Surface chirality: Origin, propagation, and amplification. **D. Wang**, T. Chen, I. Wan

9:05 – 1835. On surface tailoring of 1- and 2D supramolecular structures via hydrogen bonding. **N. Schmidt***, M. Enache, I. Georgiou, L. Maggini, D. Bonifazi, M. Stoehr

9:25 – 1836. Diverse 2D patterns in supramolecular block copolymer thin films by dip-coating. **C. Bazun***, S. Roland, C. Gamys, J. Grosrenaud, J. Vapaavuori, R.E. Prud'homme, C. Pellerin

9:45 Coffee Break

10:00 – 1837. Organized metal nanoparticle assemblies by block copolymer templating. **A.M. Ritcey**, J. Lemineur

10:20 – 1838. Multi-component 2D self-assemblies at the liquid/solid interface via optimization of multiple intermolecular interactions using designed trigonal molecular building blocks. **K. Tahara**, K. Nakatani, K. Katayama, S. De Feyter, Y. Tobe

10:40 – 1839. Competing sergeant-soldiers and host-guest chirality induction pathways at the liquid-solid interface. **K.S. Mai***, E. Ghijssens, Y. Fang, O. Ivansenko, H. Cao, K. Tahara, Y. Tobe

11:00 – 1840. Redox non-innocent ligand design for two and three electron oxidations of single-site metal centers at surfaces. **S.L. Tait***

11:30 – 1841. Supramolecular organisation on layered semiconductors and insulators. V. Korolkov, A. Summerfield, J. Kerfoot, S. Svatek, N. Besley, N. Champness, L. Yang, K. Watanabe, T. Taniguchi, **P. Beton**

Hawaii Convention Center
Halls I, II, III

Multi-scale & Synergistic Supramolecular Systems in Material and Biomedical Sciences (#357)

Organized by: S. Aoki, H. Chiu, K. Soga, N. Gianneschi, X. Bengang

Poster Session 10:00 – 12:00

1842. Wavelengths dependence of photo-induced reactions of hybrid systems of chiral Schiff base $\text{Cu}(\text{II})$ complexes. **N. Yoshida***, T. Akitsu

1843. Synthesis of self-propelled protein microtubules. **S. Kobayakawa**, T. Komatsu*

1844. Enhanced red upconversion luminescence of $\text{NaYF}_4:\text{Yb}^{3+}, \text{Er}^{3+}$ nanoparticles by Mn^{2+} doping for photodynamic therapy. **A. Omoto***, M. Kamimura, H. Chiu, K. Soga

1845. Induced CD from chiral Schiff base complexes involving azo-group to gold nanoparticles. **Y. Tsutsumi**, T. Akitsu

1846. Photodynamic activities of human serum albumin-metalloporphyrin complex. **M. Akiyama***, T. Komatsu

1847. BODIPY derivatives with fluorescence ability responding to environmental polarity and heavy metal ions. **Y. Gobo**, G.J. Richards, M. Yamamura, T. Nabeshima

1848. Synthesis of [3]rotaxanes which consist of one ring and two axles. **Y. Yamashita***, Y. Mutoh, R. YAMASAKI, T. Kasama, S. Saito

1849. Design and synthesis of light and redox reaction-driven molecular shuttles. **M. Karasaki**, A. Ota, T. Tanaka, S. Aoki

1850. Synthesis and anticancer activity of doxorubicin-loaded DNA nanotubes.

C. Yamada, M. Akiyama, T. Komatsu*
1851. Synthesis of rotacatenanes using transition metal catalysis and metal-template approach. **R. Hayashi***, K. Wakatsuki, P. Slavik, R. YAMASAKI, Y. Mutoh, T. Kasama, S. Saito

1852. Tracking of cancer metastasis in living mice with rare-earth-doped ceramic nanophosphors by over 1000 nm (OTN) near-infrared fluorescence imaging.

R. Fukushima, M. Kamimura, S. Hayashi, T. Ono, S. Murakami, H. Akiyama, F. Tashiro, K. Soga
1853. Synthesis of disaccharide nucleosides by the chemical O-glycosylation of natural nucleosides with thioglycoside donors. **T. Itoh**, T. Fukumoto, M. Kurihara, S. Saito, S. Komabiki, S. Aoki

1854. Classification of the crystal structures of $[\text{Ni}(\text{dmit})_2]$ salts of alkyl hexylidimethylammonium of various alkyl chain length.

R. Suzuki
1855. Allosteric guest binding of octaphosphonate biscavandits. **D. Shimoyama**, H. Yamada, T. Ikeda, R. Sekiya, T. Haino*
1856. Development of calixarene-based host molecules capable of binding histone tail peptide. **Y. Kajiki**, N. Tochio, J. Uewaki, S. Tate, T. Haino*

1857. Design, synthesis, and reactivity of supramolecular complexes formed by self-assembly of multinuclear zinc complexes, functionalized organic building blocks, and metals. **Y. Hisamatsu**, M. Miyauchi, K. Yoneda, Y. Miyazawa, S. Aoki

Hawaii Convention Center
316B

Materials for the Mitigation of Chemical Hazards (#388)

Organized by: J. DeCoste, G. Peterson, J. Becker, M. Biggs, L. Croll, K. Walton
Presiding: J. DeCoste

8:00 – 1858. Co-adsorption of organic and inorganic compounds on activated carbons. **P. Lodewyckx***

8:30 – 1859. Reaction analysis on the removal of aromatic sulfonates from aqueous solution by Mg-Al oxide.

M. Umetsu*, T. Kameda, T. Yoshioka
8:50 – 1860. Impregnated activated carbons vs. highly porous inorganic materials for toxic gas removal. **J. Dahn***, M. Rankin, X. Ma, J. Smith, M. McDonald, J. Romero, L. Croll

9:20 – 1861. Effectiveness of Mg-Al layered double hydroxide to remove arsenic from waste water. **M.T. Rahman***, T. Kameda, T. Yoshioka

9:40 – 1862. Modification of fibers with nanostructures for chemical defense. **T. Glover**, K. West, M. Bunge

10:10 Break

10:20 – 1863. Removal of boron and fluoride by means of adsorption process with magnesium oxide: Availability assessment. **y. yamamoto***, T. Kameda, T. Yoshioka

10:40 – 1864. Sensing, decontamination, and filtration by the multifunctional zirconium hydroxide. **G. Peterson***, J. Rossin

* Principle Author

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Hawaii Convention Center
314

Design of Innovative Photochromic Applications (#399)

Organized by: J. Abe, T. Kawai,
Y. Yokoyama, N. Branda, F. Raymo,
W. Zhu
Presiding: N. Branda

8:00 – 1865. Photochromic triangle terarylenes: Efficient photo- and electro-reactions. **T. Kawai***

8:20 – 1866. Photoswitching interlocked molecule construction and dynamic intermolecular communication.

N.D. McClenaghan*, A. Tron,
R. Bofinger, J. Thevenot,
S. Lecommandoux, J. Tucker

8:40 – 1867. Sensing or actuating with photochromic dyes. **C. Coudret***,
J. MICHEAU, J. VALLET

9:00 – 1868. Phototoxicity of photochromic diarylenethenes. **K. Uchida***,
K. Sumaru, J. Okuda, R. Kodama,
K. Morishita, T. Kanamori, S. Yokojima,
S. Nakamura

9:20 – 1869. Azobenzene photoswitching as a tool for controlling nanoscale morphology in dip-coated block copolymer thin films. **J. Vapaavuori***, J. Grosrenaud,
C. Pellerin, C. Bazuin

9:40 Break

9:55 – 1870. Photochemical control of static charge using spiropyran-functionalized polymers. **S.W. Thomas***

10:15 – 1871. Computational study of the photochromism of nitrospiropyran and merocyanine. **M. Mayes**

10:35 – 1872. Pushing the absorption of photochromic diarylenethenes into the near IR: The use of quinoidal units for a modular approach to advanced materials.

D.G. Patel, D. Carter, F. Novak, S. Myers
10:55 – 1873. Red, far-red, and near infrared photoswitches based on azonium ions. M. Dong, A. Babalhavaeji, A. Woolley*

11:15 – 1874. Single particle and ultrafast spectroscopy of new photochromic nanoparticles. **M. Sliwa***, B. Debuss, R. Bernex, C. Ruckebusch, C. Pavageau, R. METIVIER, P. Yu, H. Miyasaka, J. Abe

11:35 – 1875. Photon-working switches involving hydrogen bonds. **Y. Yokoyama***
11:55 Closing

Hawaii Convention Center
Halls I, II, III

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

Organized by: Z. Ye, C. Brown,
T. Kiguchi

Presiding: Z. Ye

Poster Session

10:00 – 12:00

1876. Electronic state of Pd nanoparticles supported on ferroelectric BaTiO₃ particle studied by in situ X-ray absorption fine structure. **T. Yoshida**, J. Kano, N. Oshime, S. Hinokuma, K. Kato, K. Nitta, m. Mizumaki, N. Ikeda, T. Fujii, T. Ohkubo, T. Ueda

1877. Temperature dependent study on the visible emission in ferroelectric nanotubes. **Y. Lee***, S. Bu

1878. Effect of silver niobate substitution on structures and electrical properties of sodium potassium niobate thin films. **X. Li***, X. Wu

1879. Phase formation, dielectric loss, and ferromagnetic properties in multiferroic PFN-PZT ceramics.

P. Amornpataratkit*, P. Jantaratana, N. Vittayakorn, S. Ananta

1880. High frequency tunable property of Ba(Zr_xTi_{1-x})O₃ films grown by reactive sputtering. **J. Kim***

1881. Ferroelectric and magnetic properties of Bi_{m+1}Ti₃Fe_{m-3}O_{3m-3} thin films.

T. Jia*, H. Kimura, Z. Cheng, H. Zhao

1882. Preparation of high-quality single crystal and spin flop of multiferroic Co₄Nb₂O. **S. Cao***, J. Zhang, W. Ren

1883. Ferroelectric properties of perovskite 0.93PZN-0.07BT ceramics fabrication from two-stage reactive sintering technique. **P.N. Pakawanit***, D.N. Ngmajarajana, D.N. Rugmai, D.N. Ananta

1884. High piezoelectricity in (K,Na)(Nb,Sb)O₃(Bi,La,Na,Li)ZrO₃ lead-free ceramics. **L. Jiang***

1885. Enhanced sensitivity in magnetoelectric laminated composite sensors based on ME nonlinearity. **J. Ma**, J. Jiao, C. Fang , H. Xu, D. Lin, S. Wang, X. Zhao, H. Luo

1886. Electrical properties of chemical solution deposited $\text{La}_{0.5}\text{Bi}_{4.0}\text{Mn}_{0.5}\text{Ti}_4\text{O}_{15}$ ($M=\text{Tb}, \text{Yb}$ and Lu) thin films. **S. Kim***, C. Raghavan, J. Kim, J. Choi

Friday Afternoon

Hawaii Convention Center
317A

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: E.E. Nesterov, M. Samal

13:00 – 1887. Excited state behavior of organic metal halide perovskite films and its influence on photovoltaic properties.

P.V. Kamat*, J. Manser

13:25 – 1888. Nanopatterning of plasmonic nanostructures for silicon surface functionalization via block copolymer self-assembly. **J.M. Burik***, F. Liu, E.J. Luber

13:50 – 1889. Real-time chemical imaging of single nanoparticles by photothermal microscopy. **B. Dragnea***

14:15 – 1890. Intermission

14:30 – 1890. Unusual electrocatalytic activity trend for $\text{Pd}_x\text{Au}_{140-x}/\text{Pt}$ ($x = 0$ to 140) core@shell nanoparticles for adsorbed CO oxidation. L. Luo, L. Zhang, G. Henkelman, **R.M. Crooks***

14:55 – 1891. Near-infrared fluorescent conjugated polymer “core-shell” nanoparticles. C.A. Chavez, T.E. Karam, L.H. Haber, **E.E. Nesterov***

15:10 – 1892. General and robust strategies to monodisperse nanoparticles and nanowires with unprecedented control over dimensions, compositions, and architectures. **Z. Lin***, X. Pang

15:25 – 1893. Graphene oxide coupled metal oxide nanosheets incorporating small organic molecules for n-type and p-type field effect transistors (FETs).

M. Samal*, N. Barange, K. Yun

15:40 – 1894. Binary nanocolloidal crystals: Preparation, characterization, and applications. **Y. Sakamoto***

15:55 – 1895. Preparation of highly dispersive hollow silica particles using vesicle template method. **H. Sakai***, T. Ohki, H. Sohma, T. Ogura, T. Endo, K. Torigoe, K. Sakai, M. Abe

16:10 – 1896. Surface enhanced NMR spectroscopy for the characterization of nanoparticle surfaces. A. Rossini, L. Piveteau, L. Protesescu, M. Valla, A. Lesage, M.V. Kovalenko, C. Copert, **L. Emsley**

16:25 – 1897. Boron- and gadolinium-rich nanoparticles for neutron capture therapy of cancer. **I. Zharov**

Hawaii Convention Center
317B

Nanocrystal Synthesis, Characterization, Assembly and Applications (#34)

Organized by: R. Tilley, S. Skrabalak, T. Hyeon, T. Nann, T. Adshiri

13:00 – 1898. Multishelled metal oxides hollow microspheres: Synthesis and applications. J. Wang, H. Ren, R. Yu, H. Zhao, **D. Wang**

13:40 – 1899. Effect of ligands on charge transfer dynamics in hybrid polymer: quantum dot photovoltaics. **R. Brutney***

14:00 – 1900. Shape, electronic structure, and steric effects of organometallic nanoparticles: A theoretical chemistry point of view and its consequence for catalysis. L. Cusinato, I. del Rosal, **R. Poteau***

14:20 – 1901. Perovskite nanocrystals: Hydrothermal synthesis and atomic-scale structural characterization. H. Wu, L. Li, S. Zhou, J. Zhu, Z. Liu, **X. Zhu***

14:40 – 1902. Luminescent silicon nanocrystals: The role of surface groups.

M. Dasog, J. Veinot*

15:00 – 1903. Molecular clusters as suprathermal in solid-state chemistry. **X. Roy***, M.L. Steigerwald, C. Nuckolls, T. Siegrist

15:20 – 1904. Rational design and synthesis of iron-oxide-based high-performance MRI contrast agents. Z. Zhao, Z. Zhou, L. Wang, **J. Gao**

15:40 – 1905. Dimensional optical property of self-assembled metallic nanoparticles.

K. Tamada*

16:00 – 1906. Controllable synthesis of metal and Metal@Semiconductor hybrid nanoparticles with highly tunable plasmonic absorption properties. **C. Li**, T. Zhang, Y. Sun, J. Li

16:20 – 1907. Revisiting an old debate: What is the origin of photoluminescence in Si nanocrystals. **R. Sinelnikov***, M. Dasog, A. Meldrum, J. Veinot

Chemistry and Applications of Graphene (#39)

Organized by: Y. Chen, R. Haddon, K. Loh

Presiding: B. Hong, J. Kong, Y. Liu, H. Zhang

13:00 – 1908. Functionalized, heterogeneous carbons: From fundamental properties to new applications.

C.W. Bielawski

13:20 – 1909. Controllable growth of high quality graphene by a chemistry vapor deposition.

L. Liu

13:40 – 1910. Time evolution of nanobubbles in graphene liquid cells: In-situ TEM study.

B. Hong*, D. Shin, J. Park, S. Cho

14:00 – 1911. Covalent modification of graphene nanoribbons with a reactive BO-DIPY complex.

A.J. Way, M. Waterland, S. Telfer, N. Lucas

14:15 – 1912. Adsorption of NO and CO molecules at the edge of graphene using DFT calculation.

A. Ishii*

14:30 – 1913. Immobilized Co(II) on porous graphene aerogels: Electrocatalytic activity.

s. bagheri

14:45 Break

15:00 – 1914. Chemical vapor deposition synthesis of graphene and related 2D materials.

J. Kong

15:20 – 1915. Warped nanographenes and soluble graphene nanoribbons.

L.T. Scott*

15:40 – 1916. Synthesis and applications of novel 2D nanomaterials.

H. Zhang*

16:00 – 1917. Green, facile, and high-yield synthesis of dimension-controllable graphene oxide nanoribbons.

W. Chiang, Y. Li

16:15 – 1918. Ge vapor assisted catalytic growth of single layer graphene on silicon dioxide substrate.

J. Lee, M. Kim, J. Lim, S. Jung, S. Hwang, D. Whang

16:30 – 1919. Direct synthesis of sub-10 nm graphene nanoribbons with smooth armchair edges on Ge(001).

R. Jacobberger, B. Kiraly, M. Fortin-Deshenes,

P. Levesque, K. McElhinny,

R. Rojas Delgado, S. Singha Roy,

A. Mannix, M. Lagally, P. Evans,

P. Desjardins, R. Martel, M.C. Hersam,

N. Guisinger, **M.S. Arnold***

Hawaii Convention Center
321A

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie

Presiding: Y. Li

13:00 – 1920. Computational approach to giant POMs and new POCATs.

C. Bo*, N. Bandeira, D. Melgar

13:25 – 1921. Hydrogen-bonded trimer of methylated molybdochelate. J. Imai, T. Ozeki, **A. Yagasaki***

13:45 – 1922. Zr-cluster substituted poly(polyoxometalates) made by synergistic structure-directing roles of lacunary fragments under hydrothermal conditions.

G. Yang*

14:05 CSMC-Flash poster-3

14:15 – 1923. All-inorganic metallacrowns by heteropolyoxovanadates.

Y. Hayashi

14:35 – 1924. Turning up the heat on redutive polyoxometalate synthesis: Benefits of COST action CM1203 (PoCheMoN).

J. Errington*, Y. Duan, W. Salomon

14:55 – 1925. Interconversion among neutral vanadium(V) oxo cluster complexes by changing the solvent systems.

S. Kodama*, N. Taya, Y. Ishii*

15:15 – 1926. Experimental and in silico investigation of Nb/Ta substituted isopolytungstates.

P.I. Molina*, P. Miro, D.J. Sures, L.N. Zakharov, T. Heine, M. Nyman*

15:35 – 1927. Synthesis and application of molybdenum oxides containing polyoxomolybdate building units.

M. Sadakane*, W. Ueda

15:55 – 1928. Niobium POM speculation in acid.

D. Park*, S. Goberna Ferron, M. Nyman, D.A. Kesler

16:15 – 1929. Inorganic-organic hybrid assembled materials based on block copolymers and polyoxometalates.

H. Wei, N. Shi, J. Zhang, X. Wan*, **J. Zhang***

16:35 – 1930. Polyoxometalate mediated oxidative transformations.

R. Neumann

Hawaii Convention Center
321B

Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101)

Organized by: F. Vetrone, S. Kohei, D. Ma, W. Huang, L. Huang, X. Peng

13:00 – 1931. Fluorescence of graphene oxides and their applications in biosensing.

N. Wu*

13:40 – 1932. Controlling the electronic properties of 2D MoS₂ through thiol functionalization.

E.P. Nguyen*, T. Daeneke, B.J. Carey, K. Kalantar-zadeh, S. Zhuiykov

14:00 – 1933. Ultrasonic modulation of photoluminescence in atomically thin molybdenum disulfide.

A. Rezki, **B.J. Carey**

14:20 – 1934. Metal-containing nanomaterials with biocompatible luminescence properties: devising luminescent nanoparticles for biomedical imaging.

K. Sorasaeene*, C. Blumenfeld,

P. Promdet, B. Rodriguez, A. Henry,

G.E. Fernandez, D. Koos, R.H. Grubbs, J. Galan-Mascaros, H.B. Gray

*** Principle Author**

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<http://pacifichem.org/onlineprogram>

14:40 – 1935. Colloidal II-VI magic-sized nanocrystals. **K. Yu***
15:20 – 1936. Dual electrochemiluminescence of BDY-PbS nanoparticles. **K. Swanick**, J. Lu, S. Wang, Z. Ding
15:40 – 1937. Modification of exciton/multi-exciton emission of quantum dots by gold nanoparticles. **J. Zhao***, S. Dey, Y. Zhou, J. Jenkins, S. Zou
16:00 – 1938. Switchable lanthanide emissive molecular monolayers. **J. Lehr***, M. Tropiano, S. Faulkner, P. Beer, J. Davis*
16:20 – 1939. White light of colloidal hybrids containing 2D crystals exfoliated from layered rare-earth (Dy^{3+} , Eu^{3+} and Tb^{3+}) hydroxides. **X. Wang***, X. Yang

Hawaii Convention Center
320 Theatre

Functional Molecular Materials and Devices (#128)

Organized by: R. Kato, H. Mori, J. Schlueter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya
Presiding: K. Kanoda, J. Takeya

13:00 – 1940. Organic charge-transfer complexes based on BTBT. T. Kadoya, Y. Kiyota, K. Iijima, T. Higashino, M. Dogishi, R. Sato, T. Kawamoto, K. Takimiya, **T. Mori***
13:25 – 1941. N-type organic semiconductors based on linearly fused N-heteroaromatics. **Q. Miao**, S. Yang, X. Xu, D. Liu

13:45 – 1942. Synthesis of substituted piperenes and its derivatives and their application to field-effect transistors. **V. Nishihara***, X. Chen, N. Chang, K. Hyodo, S. Nishinaga, Y. Okuda, H. Nonobe, J. Zhao, J. Xu, H. Mori

14:10 – 1943. Design of two-component molecular materials toward photofunctional applications. **D. Yan***

14:30 – 1944. Steering molecular orientation and strengthening π - π intermolecular interaction through perfluoroalkylation: Insights for rational design of functional molecular materials. **H. Sun***

14:50 – 1945. Synthesis, process and device fabrication of ladder polymers. **L. Fang**

15:10 – 1946. Optical control of carriers and spins in molecular materials: How to produce photomagnetic conductors from nonmagnetic insulators in an instant. **T. Naito***

15:30 break

15:45 – 1947. High-magnetic-field superconducting phase in layered charge-transfer salts. **S. Uji***, Y. Iida, K. Sugii, T. ISONO, S. Tsuchiya, N. Kikugawa, S. Tsuda, T. Terashima, H. Akutsu, J. Yamada, P. Day

16:10 – 1948. Correlations and superconductivity in organic charge transfer salts. **S. Brown***

16:35 – 1949. Observation of spatial symmetry breaking in k -(ET) $_n$ Cu $_2$ (CN) $_3$ by terahertz emission spectroscopy. **K. Itoh***, H. Itoh, N. Yoneyama, T. Sasaki, S. Iwai*

Hawaii Convention Center
322AB

Janus Materials: Design, Fabrication and Properties (#210)

Organized by: Z. Yang, S. Granick, E. Kumacheva
Presiding: C. Li

13:00 – 1950. From Janus to patchy nanoparticles: About an efficient synthesis route. A. Desert, C. Chomette, C. Hubert, J. Taveau, O. Lambert, S. Ravaine, M. Lansalot, E. Bourgeat-Lami, A. Thill, O. Spalla, L. Belloni, A. Perro-Marre, E. Duguet*

13:30 – 1951. Janus materials. **Z. Yang**

14:00 – 1952. Janus tectons for surface-confined supramolecular self-assembly: A versatile platform for the noncovalent functionalization of graphene. P. DU, D. KREHER, F. MATHEVET, F. CHARRA, A. ATTIAS*

14:30 break
14:45 – 1953. First direct observation of thermodynamically stable internally ordered Janus nanoparticles created by lipid self-assembly. N. Tran, X. Mulet, A. Hawley, C.E. Conn, J. zhai, L. Waddington, **C.J. Drummond***
15:05 – 1954. Asymmetric structures based on block copolymer brushes on silica particles. **H. Zhao***
15:25 – 1955. Design of hybrid material with water-repelling and adsorptive properties. **M. Higuchi**, S. Kitagawa*
15:45 – 1956. Number distribution of ligand chains on the surface of polymer-grafted nanoparticles. **Z. Lu**, H. Liu
16:05 – 1957. Organic-inorganic Janus composite particle through nanoscale phase separation in seeded polymerization. **D. Qiu***
16:25 – 1958. Novel radiative properties of segmented Au-Ag nanocylinders. **G. Wang***
16:45 closing remark and discussion

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Carbon Nanotubes: Preparation, Characterization and Applications (#227)

Organized by: S. Maruyama, R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: S. Maruyama, R. Weisman

13:00 – 1959. Resolution of carbon nanotube enantiomers by DNA and chiral surfactants: Common mechanism revealed. **M. Zheng**

13:30 – 1960. Fluidized-bed production of sub-millimeter-long carbon nanotubes and their application to electrochemical energy storage devices. **S. Noda***

14:00 – 1961. Chemically modified carbon nanotubes and graphene: Synthesis, assembly, and applications. **S. Kim**

14:30 – 1962. Improved photovoltaic performance of carbon nanotube-based solar cells. **K. Matsuda***

15:00 break

15:20 – 1963. Large scale sorting of single-chirality single-wall carbon nanotubes. **H. Kataura***, Y. Yamogida, X. Wei, T. Tanaka

15:50 – 1964. Environmental TEM, low-voltage SEM, and optical imaging of carbon nanotubes. **K. Jiang**

16:20 – 1965. Growth of high-density horizontally aligned SWNT arrays using Trojan catalysts. **J. ZHANG**

Hawaii Convention Center
318A

Advances in Bioinspired and Biomedical Materials (#245)

Organized by: K. Healy, Y. Ito, P. Messersmith, X. Chen, I. Kang
Presiding: P. Messersmith

13:00 Introduction

13:05 – 1966. Nitric oxide: A key player for novel target of immunotherapeutics. **Y. Nagasaki***

13:45 – 1967. Biocompatible liquid crystal elastomers with unique internal morphologies as cell scaffolds. **E. Hegmann***, A. Sharma, C. Malcuit, R. Clements, E. Freeman, L. Korley, T. Hegmann

14:05 – 1968. Microstructured polymer nanosheets for tissue engineering application. **T. Fujie***, S. Suzuki, S. Takeoka

14:25 – 1969. Bioinspired binding growth factors for regenerative medicine. **Y. Ito***

14:45 – 1970. Multiple component self-assembled peptide/polysaccharide scaffold present an antiinflammatory environment to downregulate the expression of cytokines and induces apoptosis in epithelial cancer cells. R. Li, K. Bruggeman, D.R. Nisbet, **R.J. Williams***

15:05 Coffee Break

15:20 – 1971. Construction of novel xenofree artificial extracellular matrix proteins for the culture and expansion of iPSCs. **N. Adnan***, M. Mie, E. Kobatake

15:40 – 1972. Synthetic surfaces to promote stem cell pluripotency and differentiation. **L.L. Kiessling**
16:20 – 1973. Temporally controlled bioactive 3D hydrogel scaffolds as next generation nerve grafts. **A. Badea**, J.M. McCracken, E.G. Tillmaand, S.S. Rubakhin, J.V. Sweedler*, R.G. Nuzzo*

16:40 – 1974. Novel cytoplasm transplantation method by microdevice. **K. Wada**, K. Hosokawa, Y. Ito, Maeda*

Hawaii Convention Center
318B

Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials (#309)

Organized by: A. Smirnov, S. Bottle, R. Tamura
Presiding: I.J. berliner, A. Smirnov

13:00 Introductory Remarks - Alex I. Smirnov

13:05 – 1975. Design and synthesis of nitroxide radicals for biophysical and biomedical applications. **A. Rajca***

13:35 – 1976. Access to local surface water dynamics and structure by spin labeling and Overhauser DNP. **S. Han**

14:05 Session Break

14:20 – 1977. Mono- and biradical nitroxide cysteine-specific labels for structural biology of membrane protein by solid-state NMR and DEER spectroscopy. **A. Smirnov**, M. Voynov, S. Milikisityants, S. Wang, R. Munro, M. Donohue, L. Brown, T. Smirnova, V. Ladizhansky

14:50 – 1978. Bifunctional spin labeling of muscle proteins: Accurate rotational dynamics, orientation, and distance by EPR. **A. Thompson**, B.P. Binder, J.E. McCaffrey, B. Svensson, D.D. Thomas*

15:20 – 1979. Nitroxide-tagged platinum(II) compound enables identification of DNA G-quadruplex binding mode. **X. Zhang**, C. Xu, Z. Mao, **P.Z. Qin***

15:40 – 1980. Probing the electrostatics of biointerfaces by EPR of spin-labeled phospholipids with pH-dependent EPR spectra. **M.A. Voynov**, A. Koolivand, C. Scheid, I. Kirilyuk, A. Marek, A. Smirnov

16:00 – 1981. pH-sensitive nitroxide probes to probe electrostatics and proton gradients in membrane protein systems. **T. Smirnova***, M. Voynov, A. Smirnov

Hawaii Convention Center
319B

Membranes and Nanotechnologies for Energy and Environment Applications (#317)

Organized by: H. Park, B. Freeman, B. McCloskey, J. McGrath, A. Hill, A. Higuchi, Y. Lee
Presiding: H. Park

13:00 – 1982. New approach for scientific research on RO membrane. **M. Kimura***, T. Ogawa, K. Nakatsui, T. Sasaki

13:30 – 1983. Construction of biomimetic asymmetric membranes and application of them in the field of energy and environment. **L. Wen**, L. Jiang

13:50 – 1984. Complexation induced phase separation: Preparation of composite membranes with a nanometer thin dense skin loaded with metal ions. **L. Villalobos***, K. Peinemann

14:10 – 1985. Correlating transport and stability of ion-exchange membranes through nanostructure. **A. Kusoglu**, a.z. weber

14:30 – 1986. Design and synthesis of membranes for artificial photosynthesis. **N.A. Lynd**

14:50 – 1987. Polymer electrolytes with high lithium ion transference numbers. **B.D. McCloskey***

15:20 – 1988. Ionic diode membrane for salinity gradient power generation. **W. Guo***, L. Jiang

15:40 – 1989. Ion transport structure/property relationships in charged polymer membranes. **G.M. Geise***

16:00 – 1990. Self-assembled nanoporous nanoparticle network films for membrane applications. N. Kwon, H. Lee, H. Park, **B. Lim***
16:20 – 1991. Template-free hydrothermal synthesis and high alcohol selectivity of silicate-1 membranes with nanosize seed. **C. Cho***, S. Hu

16:40 – 1992. Membrane migration method for the purification of adipose-derived stem cells from fat tissue through synthetic porous membranes. **A. Higuchi**, S. Kumar, A. Alarfaj, M. Munusamy

Hawaii Convention Center
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Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei, A. Wee, W. Chen, P. Weiss
Presiding: C. Wang

13:00 – 1993. On-surface host-guest chemistry of planar pyridine macrocycles with organic cations. **Y. Tobe***

13:30 – 1994. Supramolecular assembly through ion-dipole interaction. **Y. Kim***

14:00 – 1995. Desorption rates and energy of desorption measurements at the solid solution interface. **K. Hipp***, U. Mazur, A. Bhattachari

14:30 – 1996. Clocking surface-reaction by the observed in-plane rotation of a product. **K. Anggra**, A. Chatterjee, F. Cheng, K. Huang, L. Leung, J. Polanyi

14:50 – 1997. Molecular quasicrystals: Penrose tiling with molecules. S.J. Narn, G. Waterhouse, D.C. Ware, **P.J. Brothers***

15:10 Coffee break

15:20 – 1998. Hydrogen-bonding in control of supramolecular ordering of organic semiconductors. **C. Fu***, H. Lin, J. Macleod, A. Kravev, F. Rosei, D. Perepichka

15:40 – 1999. Tuning the self-assembly of 5-amino-[6]helicene on solid surfaces. H. Ascolani, M.W. van der Meijden, L.J. Cristina, J. Gayone, R.M. Kellogg, J.D. Fuhr, **M. Lingenfelder***

16:00 – 2000. Toward spatio-temporally resolved chemistry: The role of surface confinement. **S. Hecht***

16:30 – 2001. Self-assembly of organics on carbon surfaces and applications for electronic devices. **Z. Bao***

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316C

Fundamentals and Applications of Nanomaterials for Energy Technologies (#348)

Organized by: S. Jin, G. Yu, T. Minegishi, S. Maldonado, J. He
Presiding: S. Maldonado, G. Zheng

13:00 – 2002. Publishing in Wiley materials science journals. **J.R. Oliveira***

13:30 – 2003. Semiconductor heterostructures for energy conversion, storage, and bio-interfaces. **G. Zheng***

14:00 – 2004. Charge separation in heterostructured nanoparticles. **T. Teranishi***

* Principle Author

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- 14:30 – 2005.** Exotic Au nanostructures: Structure solution, properties, and applications. **Y. Han**
- 15:00** Break
- 15:15 – 2006.** Can surface plasmon promote energy conversion effectively. C. Zhan, Y.F. Huang, **Z. Tian**
- 15:45 – 2007.** Synthesis of chemically modified graphene materials for energy applications. **G. Shi***
- 16:15 – 2008.** SURMOFs/CNCs as tuneable photonic and optoelectronic materials for light harnessing and solar energy applications. **E. Redel**
- 16:30 – 2009.** Nanograined half-Heusler Ti-NiSn for thermoelectric applications. **M. Buffon**, R. Seshadri
- 16:45 – 2010.** Aerogels as novel matrices and spacers of ultralow thermal conductivity for applications in nano-enabled thermoelectrics. **N. Mishra**, M. Jaime, C. Hamilton, J. Torres, J. Hollingsworth

Hawaii Convention Center
316B

Multi-scale & Synergistic Supramolecular Systems in Material and Biomedical Sciences (#357)

Organized by: S. Aoki, H. Chiu, K. Soga, N. Giannessi, X. Bengang
Presiding: K. Soga

- 13:00** Opening remarks
- 13:05 – 2011.** Supramolecular systems constructed of porous solids and guest inclusions for energy and environmental applications. **M. Suh***, D. Lim, H. Park, S. Sung
- 13:30 – 2012.** Highly diastereoselective guest encapsulation by self-assembled disymmetric capsule. **T. Haino***
- 13:55 – 2013.** On-colloid supramolecular assembly of nanoparticle growth templates. **J.E. Millstone**
- 14:15 – 2014.** Nanosecond charge carrier lifetimes in hierarchical donor-acceptor supramolecular polymer films. **A.B. Braunschweig**, A.M. Scott, C.X. Guzman, S. Yamazaki
- 14:35 – 2015.** Odd-even effect in the crystal structure of $[Ni(dmit)_{2}]$ salt of alkylammonium enhanced by substitution of end methyl group with phenyl group. **K. Miyamura***, M. Saeki

- 14:55** Break
- 15:00 – 2016.** Design of functional glycomaterials and the biological consequences of multiscale glycans presentation at cellular boundaries. **K. Godula***
- 15:20 – 2017.** New polymer-MOF hybrids built from the ground up. **S. Cohen***, S.A. Miller
- 15:40 – 2018.** Reversible anion transport and biological properties using host-guest competitive processes. **J. Gravel**, A.R. Schmitz*
- 16:00 – 2019.** Design and synthesis of luminescent cyclometalated iridium(III) complexes for material and biomedical science. **S. Aoki***, Y. Hisamatsu, A. Kando, N. Suzuki, A.A. Masum, H. Tanaka, S. Kumar
- 16:25 – 2020.** Dipyrrom-typical-element complexes with unique and responding functions. **T. Nabeshima***

Hawaii Convention Center
319A

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

Organized by: Z. Ye, C. Brown, T. Kiguchi
Presiding: Z. Ye

13:00 Opening

13:05 – 2021. Spin and lattice dynamics in multiferroic $BiFeO_3$. G. Xu*, **Z. Xu**, J. Schneeloch, j. Wen, C. Stock, P.M. Gehring, M. Stone, M. Matsuda, B. Winn, T. Berlijn, W. Ku, G. Gu, S. Shapiro, R. Birgeneau, T. Ushiyama, Y. Yanagisawa, Y. Yomioka, T. Ito

- 13:30 – 2022.** Toward enhancement of magnetoelectric performance in spin-driven ferroelectrics. **T. Kimura***
- 13:55 – 2023.** Raman spectroscopy and photovoltaic responses of doped $BiFeO_3$ multiferroic ceramics. **C. Tu**, C. Lin, V.H. Schmidt, R. Chien
- 14:10 – 2024.** Multiferroic and magnetoelectric nanocomposites for data processing. **W. Kleemann***, P. Borisov, C. Schmitz-Antoniak, L. Herrichs, H. Wende
- 14:25 – 2025.** Noncentrosymmetric metals: A new materials class for artificial multi-ferroic design. **J. Rondinelli***
- 14:45** Break

- 14:55 – 2026.** Electrically controlled non-volatile switching of magnetism in multiferroic heterostructures via engineered ferroelastic domain states. **M. Liu***, T. Nan, N. Sun, Z. Ye
- 15:20 – 2027.** Magnetic control of ferroelectric polarization in a self-formed single magnetoelectric domain of multiferroic $Ba_2NbFe_3Si_2O_{14}$. **Y. Choi***, N. Lee
- 15:35 – 2028.** Effect of strain on ferroelectric field effect in strongly correlated oxide $Sm_{0.5}Nd_{0.5}NiO_3$. L. Zhang, J. Gardner, V. Singh, X. Hong*
- 15:50 – 2029.** Strong ferrimagnetic-dielectric coupling in multiferroic Lu_2CoMnO_6 single crystals. **N. Lee***, H. Choi, Y. Jo, Y. Choi
- 16:05 – 2030.** Multiferroic perovskite nanoparticles: Microwave-hydrothermal synthesis, structural characterization, and visible-light photocatalytic properties. H. Wu*, L. Li, S. Zhou, J. Zhu, Z. Liu, X. Zhu*
- 16:20 – 2031.** Spin-lattice coupling in a paraelectric antiferromagnet $EuTiO_3$. **H. Cao***, J. Hong, O.A. Delaire, J. Yan
- 16:35 – 2032.** Multifunctional $BiFeO_3$ - $ATiO_3$ [A: Pb, Ba] thin films: Chemical composition modification and electrical and magnetic properties. **W. Sakamoto***, Y. Ito, A. Iwata, D. Maeda, N. Makino, T. Yogo

Friday Evening

Hawaii Convention Center
317A

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: V. Ksenofontov

- 19:00 – 2033.** Magnetic properties of iron oxide nanoparticles imbedded in a coordinating polymer matrix. **V. Ksenofontov***, S. Shylin, M. Tahir, F. Liqat, P. Daniel, W. Tremel
- 19:15 – 2034.** Recent advances in the synthesis of organosoluble thiolate-protected metal nanoparticles. **P.J. Goletti***, J. Sidletsky, B. Root
- 19:30 – 2035.** Utilizing electron transfer effect to enhance the chemical stability of Ag within the shell of nano-heterostructured particles with Au or Pt in the core. **A.T. Dao***, D.M. Mott, S. Maenosono
- 19:45 – 2036.** Magnetorheology of core-shell structured carbonyl iron/polystyrene foam microparticles suspension with enhanced stability. **Y. Seo***, W. Chuan
- 20:00 – 2037.** Synthesis of organic-inorganic hybrids using various alkoxy silane-functional polymer precursors via hydrolytic and non-hydrolytic polymerization process. **J. Kim***, N. Kim
- 20:15 – 2038.** Improvement of the thermal stability of mesoporous titania with crystalline framework using silane coupling agent and pluronic surfactants. **T. Endo***, T. Tojo, K. Torigoe, K. Sakai, M. Abe, H. Sakai
- 20:30 – 2039.** Removal of petroleum crude oil spill from sea water using high magnetization antimicrobial biocompatible magnetite nanoparticles. a.m.tta, **h.a. al-lohedian**

Hawaii Convention Center
Halls I, II, III

Chemistry and Applications of Graphene (#39)

Organized by: Y. Chen, R. Haddon, K. Loh
Presiding: S. Bak, Y. Chen, Y. Huang

Poster Session

19:00 – 21:00

- 2040.** Preparation of water-dispersible few-layer graphenes via edge-only oxidation, followed by shear-induced exfoliation. **T. Yoon***, J. Lee, H. Yoon
- 2041.** Simple preparation of reduced graphene oxide encapsulation film for organic photovoltaic device. **T. Kim**, J. Kang, S. Yang, S. Sung, Y. Kim, C. Park

- 2042.** Fabrication of few-layer graphene sheets using a serious linear diamino alkanes. **J. Li***, J. Li*

- 2043.** Wafer-scale nanoporation of single-layer graphene by arrayed Pt nanoparticles. **m. park***

- 2044.** Fluorination of nanodiamond/nanographene-shell structure. **K. Kogane**, H. Touhara, Y. Hattori, K. Takai*

- 2045.** Correlation between spin magnetism and chemical activity in graphene oxide/nanographene. **T. Yamashina**, T. Isaka, K. Inoumi, Y. Matsuo, K. Takai*

- 2046.** Control the bandgap of graphene quantum dots with functional groups. **S. Bak**, H. Lee*

- 2047.** Enhanced sensitivity of DNA sensing by surface-passivated graphene oxides. **B. Lee***, M. Lee, Y. Kim, B. Hong*

- 2048.** Mechanical flexibility and electrical conductivity of graphene films synthesized by plasma treatment. **M. Ishihara**, Y. Okigawa, T. Yamada, M. Hasegawa

- 2049.** Electrocatalytic properties of Pt or Pt-Ru alloy nanoparticles on modified carbon nanomaterials by electrodeposition methods. **H. Yoshitake**, E. Inami, Z. Wang, H. Ogata

- 2050.** Direct observations of graphene dispersed in solution by FRET-TIR microscopy. **Y. Matsuno**, Y. Sato, M. Sano*

- 2051.** STM observation of graphene oxide reduced by vacuum ultraviolet irradiation. **H. Nakamoto***, Y. Tu, O.P. Khatri, T. Ichii, T. Utsunomiya, S. Kurokawa, H. Sugimura

- 2052.** Tuning molecular adsorption kinetics in graphene by gate-bias voltage. **T. Umehara**, K. Takai

- 2053.** Bromine adsorption effects on epitaxial graphene. **K. Nakamoto**, K. Takai, T. Akatsu

- 2054.** Liquid crystal property driven selective seiving of graphene oxide and its electrochemical properties. **K. Lee**, S. Kim*

- 2055.** Application of graphene to the removal of $Pb(II)$ and $Cd(II)$ cations from aqueous solutions. **S. Hemidouche**, L. Boudriche, A. Boudjemaa, **S. Hamoudi***

- 2056.** Immobilization and photoreduction of graphene oxide on hydrogen-terminated silicon. **S. Kokufuta***, Y. Tu, T. Ichii, T. Utsunomiya, H. Sugimura

- 2057.** Modeling of the adsorption of aromatic organic compounds by graphene oxide based on its surface structure. **H. Yang***

- 2058.** Matrix-free LDI-TOF mass analysis of small molecules using converted graphene surfaces. **H. Kang**, H. Yun, S. Lee, W. Yeo*

- 2059.** Thermal conduction and dissipation application of polymer composites including graphene. **W. Oh**

- 2060.** Structural characterization of graphene based morphologies for cathode application in fuel cells. **K. Lehmann***, O. Yurchenko, G. Urban

- 2061.** Highly efficient nucleic acid drug delivery by graphene oxides. **J. Yoo**, E. Jeong, H. Lee, B. Hong

- 2062.** Graphene-enhanced conductivity and shape modulation of ionic hydrogel. **Y. Kim***, B. Hong*

- 2063.** Preparation of graphene oxide/polyvinyl alcohol microcomposites and their thermal conducting properties. **S. Kim**, Y. Azuma, Y. Kuwahara, T. Ogata, S. Kurihara

Hawaii Convention Center
321A

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie
Presiding: D.C. Crans

- 19:00 – 2064.** Computational study of the water oxidation mechanism catalyzed by the polyanion $[Co_4(H_2O)_2(XW_9O_{34})_3]^{10-}$ ($X = P^{5+}, V^{5+}$). **J. Soriano-Lopez***, J. Galan-Mascaros, J. Carbo, J. Poblet, D.G. Musaev, C.L. Hill

- 19:20 – 2065.** Natural born catalysts: The great POM beauty. **M. Bonchio***

- 19:40 – 2066.** Water-oxidation catalysis starting with cobalt polyoxometalates: Addressing the challenging, "who's the true catalyst" question. **R.G. Finke***

- 20:00 – 2067.** Polyoxometalate catalyst design for water oxidation and reduction. **G.R. Patzke**

- 20:20 – 2068.** Catalytic water oxidation with cobalt-containing POMs: Processing and activity in the solid state and into plastic thin films. **J. Galan-Mascaros**, M. Blasco-Ahicart, J. Soriano-Lopez

- 20:40 – 2069.** Polyoxometalate catalysts for solar fuel production. **C.L. Hill***, H. Lv, S.M. Lauinger, Q. Yin, J. Vickers, E.N. Glass, J. Sumilner, Y.V. Geletti, D.G. Musaev, T. Lian

Hawaii Convention Center
320 Theatre

Functional Molecular Materials and Devices (#128)

Organized by: R. Kato, H. Mori, J. Schlüter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya
Presiding: S. Lo

- 19:00 – 2070.** Questioning of superconductivity in aromatic hydrocarbons.

- S. Heguri***, M. Kobayashi, K. Tanigaki

- 19:20 – 2071.** Synthesis and physical properties of a chiral donor with reduced π -electron system. **N. Nishikawa***, T. Watanabe, Y. Yoshimura

- 19:40 – 2072.** Molecular design and electronic properties of TTF- and TPP-based salt-bridge conductors. **Y. Kobayashi***, T. Teranishi, S. Sumi, Y. Matsushita, H. Iwai, A. Tanaka

- 20:00 – 2073.** In-operando studies of ultra-thin film OFETs using soft X-ray microspectroscopic probes. **R.H. Fink**, X. Du, B. Rosner, P. Warnick, N. Pilet

- 20:20 – 2074.** Controlling the stereochemistry and regularity of butanethiol self-assembled monolayers on Au(111).

- J. Reimers***, J. Yan, R. Ouyang, P.S. Jensen, E. Ascić, D. Tanner, B. Mao, J. Zhang, C. Tang, N.S. Hush, J. Ulstrup

- 20:40 – 2075.** Exotic properties of nanoscale molecular charge transfer clusters. **S.W. Hla***

*** Principle Author**

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Hawaii Convention Center
Halls I, II, III

Janus Materials: Design, Fabrication and Properties (#210)

Organized by: Z. Yang, S. Granick,
E. Kumacheva

Poster Session
19:00 – 21:00

- 2076.** Construction of hierarchical structured hydrogel film as scaffold for 2D and 3D cell co-culture. F. Zhu, Y. Chen, S. Yang, Q. Wang, F. Liang, X. Qu*, Z. Yang
- 2077.** Experimental and theoretical study on lateral buckling of Janus nanowalls. H. Yoon, W. Lee*
- 2078.** Novel method to fabricate anisotropic highly porous silica core/shell microspheres. J.K. Maisch, H.A. Mayer
- 2079.** Janus hollow spheres. F. Liang*, Z. Yang
- 2080.** Synthesis and application of anisotropic particles. L. Huarong*, F. Wang*
- 2081.** Templated synthesis of paramagnetic Janus nanotubes from PDVB nanotubes. H. Zhang, F. Liang, Q. Wang, Z. Yang*
- 2082.** Crosslinked hollow epoxy resin microspheres with single hole in their shells. J. Liu, F. Liang, Z. Yang*
- 2083.** Janus polymeric nanosheets. Q. Wang, Z. Yang*
- 2084.** Facile preparation of Janus silica nanoparticles by SI-ARGET ATRP in aqueous disperse systems. X. Dong*, W. Zhang, J. He*

Hawaii Convention Center
315

Carbon Nanotubes: Preparation, Characterization and Applications (#227)

Organized by: S. Maruyama,
R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: S. Maruyama, M. Zheng

19:00 – 2085. Carbon nanotube thin-film static random access memory.
M.C. Hersam*

19:30 – 2086. Scalable assembly and alignment of semiconducting carbon nanotube arrays for high performance field effect transistors. G. Brady, H. Evensen, Y. Joo, A. Albrecht, M. Shea, P. Gopalan, M.S. Arnold*

19:50 – 2087. Single-walled carbon nanotubes as hole transport layer and electrode for solar cells. S. Maruyama*

Hawaii Convention Center
318A

Advances in Bioinspired and Biomedical Materials (#245)

Organized by: K. Healy, Y. Ito,
P. Messersmith, X. Chen, I. Kang
Presiding: P. Messersmith

19:40 – 2088. Poly(catecholamine): A new class of bioinspired adhesive polymers. H. Lee*

19:40 – 2089. High performance mussel-inspired adhesives of reduced complexity. K. Ahn*, S. Das, R. Linstadt, Y. Kaufman, N. Martinez, R. Mirshafiani, E. Kesselman, Y. Talmon, B.H. Lipshtz, J.N. Israelachvili, J. Waite

20:00 – 2090. Hydrogen peroxide generation and biocompatibility of mussel adhesive moiety. H. Meng, B.P. Lee*

20:20 – 2091. Mussel-inspired cell-adhesion peptide coated PDMS microspheres for enhanced vocal fold augmentation of paralyzed larynx. S. Kwon*

20:40 – 2092. Rapid fabrication of hierarchical tissues by reeling-based cell fiber assembly. S. Iwanaga*, T. Okitsu, S. Takeuchi

Hawaii Convention Center
Halls I, II, III

Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials (#309)

Organized by: A. Smirnov, S. Bottle,
R. Tamura
Presiding: S.E. Bottle, A. Smirnov,
R. Tamura

Poster Session
19:00 – 21:00

- 2093.** Preparation and magnetic properties of all-organic nitroxide biradical liquid crystals. K. Taguchi*, K. Suzuki, S. Devendra, Y. Takemoto, S. Takaoka, Y. Uchida, D. Mazhukin, I. Grigor'ev, R. Tamura
- 2094.** Mapping of chemical environment by paramagnetic probes using Overhauser enhancement. A.V. Samoilov*
- A. Bobko, W. Takahashi, I. Dhimitrak, O. Efimova, J.L. Zweier, V.V. Khramtsov
- 2095.** Spectral-spatial rapid scan EPR imaging with nitroxide spin probes. M. Tseytin*, J.R. Biller, D.G. Mitchell, H. Elajaili, G.A. Rinard, R.W. Quine, G.M. Rosen, J.P. Kao, L.A. Buchanan, J. McPeak, Y. She, G.R. Eaton, S.S. Eaton

- 2096.** Preparation and magnetic properties of metal-free magnetic nanoemulsions encapsulating nitroxide radicals. K. Nagura*, Y. Takemoto, Y. Uchida, S. Shimono, T. Kato, J. Yamauchi, R. Tamura
- 2097.** Theoretical investigation of the efficiency of electron propagating through molecules using biradical molecular wires by DFT calculations. S. Nishizawa, J. Hasegawa, K. Matsuda*
- 2098.** Singlet oxygen topology on the nanoscale. M. Forbes

- 2099.** Studies on magnetic properties of bis(nitronyl nitroxide) and bis(minonitroxide)-substituted azulenes. M. Haraguchi, E.V. Tretyakov, S. Suzuki, M. Kozaki, K. OKADA*
- 2100.** Studies on magnetic properties of trinuclear gold(I) complexes bearing imino nitroxide radicals. T. Wada, S. Suzuki, M. Kozaki, d. shiom, k. sato, t. takui, K. OKADA*
- 2101.** Stable boronated triaryl methyl radicals for the measurement of glucose, hydrogen peroxide, and peroxy nitrite by electron paramagnetic resonance. B. Driesschaert*, A. Bobko, J.L. Zweier, V.V. Khramtsov
- 2102.** 6-Oxoverdazyl polymers. J.A. Paquette, J.T. Price, C.S. Harrison, R.R. Maar, J.B. Gilroy*

Hawaii Convention Center
Halls I, II, III

Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei,
A. Wee, W. Chen, P. Weiss

Poster Session
19:00 – 21:00

- 2103.** 3D printing of functional nanostructures. J. Zhao, L. Swartz, A. Sulkanen, J. Frommer, G. Liu*
- 2104.** Unique adsorption behaviors of carboxylic acids at rutile TiO₂(110). Y. Yu, X. Gong*
- 2105.** Dual component grafting of HOPG: Toward large scale morphology control. T. Phan, Y. Fujita, H. Van Gorp, J. Greenwood, T. Huynh, Z. Li, O. Ivashenko, H. Ujii, S. De Feyter*
- 2106.** Architectural control of surface properties and morphology of fluoromethacrylate copolymers. H. Peng*, A. Chen, I. Blakey, K. Jack, A. Whittaker

- 2107.** Supramolecular interaction of side chain crystalline polymer and interaction function with polyethylene and polytetrafluoroethylene. S. Yao*, A. Maeda, H. Obuchi, M. Yamasaki, R. Nakano, H. Sekiguchi

2108. Structure and disassembly of a biominerization protein on a biologically relevant surface. W. Shaw, B. Tarasevich, J. Tao, G. Buchko, J. De Yoreo

2109. Development of surface control technique by the photoresponsive self-assembled monolayer toward organic field-effect transistors. T. Konishi, K. Yamaguchi*

2110. Construction of calix crown-containing polymer nanosheet for capturing cesium ion. K. Sato*, G. Noguchi, K. Asao, A. Murata, T. Fujie, Y. Nagase, S. Takeoka

2111. Self-assembled structures of alkyl-derivatized diketopyrrolopyrrole pigment at surface and in crystal. A. Honda*, Y. Tamaki, K. Miyamura

2112. Chemical functionalization of 2D surfaces with nonbiofouling polymer coating. S. Ko, G. Han, J. Lee*

2113. STM observation of nucleation-elongation process of surface-confined self-assembly based on hydrogen bond network via amide or urea group. N. Nishitani, T. Hirose, K. Matsuda*

2114. Competitive adsorption of water and surfactants at solid/ion liquid interfaces. K. Okada*, T. Misuno, T. Endo, K. Sakai, M. Abe, H. Sakai

2115. Scanning tunneling microscopy investigation on nanoparticle packing driven by line tension. S.L. Riechers*, W. Lin, S. Wang, J. Zhang, Q. Zhong, S. da Rocha, G. Liu

2116. Orientation and photofunctional properties of the thin films of oligothiophene derivatives. H. Urino, A. Kodaira, C. Pac, H. Moriyama*

2117. Arrangement and reorganization of gold nanoparticles on nanolines prepared by scanning probe lithography on indium tin oxide surface. J. Yang*, T. Ichii, K. Murase, H. Sugimura

2118. Construction of 2D cyclic array of zinc porphyrin derivative and binding of fullerene. K. Iritani, K. Tahara, Y. Tobe*

2119. Self-assembled structures of alkoxy-derivatized Ni(II)-salen complex investigated by scanning tunneling microscopy. K. Morita*, A. Honda, Y. Tamaki, K. Miyamura

2120. Desorption kinetics at the solution-graphite interface: An STM study. A. Bhattachari, K. Hippis, U. Mazur

2121. Thermally activated transition with accompanying dimensional variation: Squaric acid on Au(111). K. Ueji*, J. Jung*, J. Oh, K. Miyamura, Y. Kim*

Hawaii Convention Center
Halls I, II, III

Fundamentals and Applications of Nanomaterials for Energy Technologies (#348)

Organized by: S. Jin, G. Yu, T. Minegishi, S. Maldonado, J. He
Presiding: J. He, S. Maldonado, T. Minegishi

Poster Session
19:00 – 21:00

2122. Hydrogen evolution from water using Cu_n(Ga)Se₂ photocathodes modified with nanometer-thick conductor layers. T. Minegishi, H. Kumagai, H. Kaneko, K. Domen*

2123. Rh_{2+y}Cr_yO₃-loaded LaMg_{1/3}Ta_{2/3}O₂N as a hydrogen evolution photocatalyst in Z-scheme overall water splitting. Z. Pan*, T. Hisatomi, C. PAN, Q. Wang, T. Takata, K. Domen

2124. Semiconductor photoanodes sheathed with ultrathin nanolayers of double hydroxides for photoelectrochemical oxidation of water. X. Xiang, W. He

2125. Photovoltaic performance of solar cells sensitized with ZnSe-AgInSe₂ solid solution quantum dots. H. Shibakawa, Y. Douke, T. Kameyama, M. Kawaraya, H. Segawa, S. Kuwabata, T. Torimoto*

2126. Effect of capping agent on CdS nanoparticlesstructure for quantum dots-sensitized solar cells. C. Kusumawardani*, A.K. Prodjosantoso, K.H. Sugiyarto

2127. High cycling performance of SiO₂ coated on multiwall carbon nanotubes for anode material of lithium-ion battery. Q. Sun, X. Liu, W. Yiu, A. Djurišić, M. Xie, A. Ng, W. Chan

2128. Improvement in the energy storage properties of ZnO based LIB anode by precursor treatment. X. Liu, F. Liu, Q. Sun, M. guo, A. Djurišić, A. Ng, M. Xie, W. Chan

2129. Microstructures of Si-SiO_x core-shell nanoparticles as an anode material for Li-ion battery. B. Jang*, J. Lee, J. Koo

2130. Li₂Ti₅O₁₂/Graphene nanoribbon composites as anodes for lithium-ion batteries. P.A. Medina*, H. Zheng, B.D. Fahrlman

2131. High energy mechanical milling route to indium selenide carbon nanocomposites with promising electrode functionality. S. Oh*, S. Hwang

2132. Development of the direct glucose fuel cell with a high power density. M. Takahashi*, K. Iwabata, K. Torigoe, Y. Kanai, T. Ruike, K. Sakaguchi, H. Sakai, M. Abe

2133. Growth and characterization of lithium ion conductor La_{2/3-x}Li_xTiO₃ single crystals. C. Kobayashi*, M. Nagao, S. Watauchi, I. Tanaka

2134. Self-assembled polythiophene-fullerene-single-walled carbon nanotube ternary nanocomposites showing p heterojunction. M. Kawamoto*, Z. Li, A. Furube, K. Seki, K. Tajima, Y. Ito

2135. Imaging of time-dependent changes of hydrophilicity and its inhomogeneity on a titanium dioxide film induced by UV irradiations studied by the newly developed NIR camera (Comprovision). I. Tanabe*, D. Ishikawa, D. Furukawa, M. Ishigaki, T. Goto, T. Morishima, T. Okuno, Y. Ozaki

2136. ZnO – organic molecule hybrid interlayer for transparent organic tandem photovoltaic. C. Chi, H. Chang, C. Shih, C. Ma, B. Huang, Y. Tai*

2137. Facile preparation of PEDOT/GO hybrid composites for supercapacitors. Y. Sulaiman*, N. Azman, H. Lim

2138. Vanadium oxide nanostructures for smart window applications. Y. Jung, J. Han, S. Chung*

2139. In situ solid-state NMR studies on the size dependency of hydrogen storage property of Pd nanoparticles under controlled hydrogen gas pressure. S. Dekura*, H. Kobayashi, R. Ikeda, M. Maesato, Y. Kubota, H. Kitagawa

2140. Control of relative geometry between porphyrins accumulated at phase segregation interface of normally oriented cylindrical nanostructure. J. Takehisa, G. Akimoto, S. Asaka*

2141. Electrically reinforced polymer composites of PMMA with MWCNT-PANI. T. Hussain*, F. Bashir, A. Samad, A. Mujahid, K. Shehzad, M.H. Raza

2142. Synthesis of CIS (CuInSe₂) solar cell in aqueous phase under room temperature. H. Takahashi*, H. Fujiki, M. Takagi, S. Yokoyama, K. Tohji

2143. Investigating the effect of grain size on the nanostructured chalcopryte thermoelectric material. M.S. Singh*, K. Gupta, S. Nishino, M. Miyata, D. Mott, M. Koyano, S. Maenosono*

* Principle Author

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- 2144.** Structure dependence of anharmonic effects in thermoelectric materials.
T. Hata*, R. Jono, K. Yamashita
- 2145.** Copper manganese sulfide nanoparticles for a sustainable thermoelectric material.
K. Gupta, . Singh, D.M. Mott, M. Koyano, S. Maenosono*
- 2146.** Synthesis of Sn-Bi-Te ternary thermoelectric alloy nanoparticles by controlling the metal complexes condition in aqueous solution.
H. Takahashi*, **S. Kon**, S. Yokoyama, K. Tohji
- 2147.** Bubble propelled nanomotor based on aggregation of thiol-modified Pt/Au nanorod.
R. Katogi, I. Shitanda, M. Itagaki, Y. Hosoi
- 2148.** Microwave-assisted synthesis of platinum-ruthenium-cobalt-graphene catalysts for fuel cells.
L. Tamasauskaitė-Tamasiunaite*, T. Kaveckas, A. Balciunaite, M. Semasko, V. Kepeiniene, J. Vaiciuniene, A. Drabavicius, E. Norkus
- 2149.** Kinetics of sodium borohydride hydrolysis catalyzed by cobalt with a fiber structure decorated with gold or platinum nanoparticles.
E. Norkus*, A. Zabielaite, I. Stalnioniene, S. Lichiusina, D. Simkunaite, B. Simkunaite-Stanyniene, A. Matusevičiute, A. Selskis, L. Tamasauskaitė-Tamasiunaite
- 2150.** First principles study of adsorption mechanisms of lithium oxides (Li_xO_2) on a graphene-based electrode.
J. Lee, H. Moon, Y. Yoon, S. Kang, I. Kim, **S. Lee***

- 2151.** Synthesis and characterization of fullerene derivatives with an alkyl chain spacer in organic photovoltaic devices.
Y. Kuda, K. Abe, H. Lee, J. Lee, J. Jang, C. Pac, H. Moriyama*
- 2152.** Novel graphene-based porous materials: Synthesis and applications.
Y. Li, G. Shi
- 2153.** Facile strategy for robust graphene films in a large scale.
m. zhang*, G. Shi
- 2154.** Pure surface plasmon resonance induced photocurrent.
C. Zhan, B.W. Liu, S. Hu, B. Ren, Z. Tian
- 2155.** First principles study of the Na adsorption mechanisms on graphene and graphene oxide.
H. Moon, J. Lee, H. Lee, S. Kwon, I. Kim, **S. Lee***

Hawaii Convention Center
319A

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

- Organized by: Z. Ye, C. Brown,
T. Kiguchi
Presiding: J.L. Jones
- 19:00 – 2156.** Design of new tetrahedral ferroelectric system.
M. Itoh*, Y. Hamasaki, S. Yasui, T. Taniyama, A. Konishi, H. Moriwake
- 19:25 – 2157.** Multiferroic perovskite structure and function design from the first principles.
W. Ren*
- 19:40 – 2158.** Magnetic field induced unidirectional transmission of THz light in multiferroics.
T. Room*
- 19:55 – 2159.** Interfacial flexoelectricity in oxide superlattices.
H. Xu*, A. Plymll
- 20:10 – 2160.** New ferroelectrics and antiferroelectrics by design.
K.M. Rabe*

Hawaii Convention Center
Halls I, II, III

Application of Luminescent Materials for Radiation Detection (#442)

- Organized by: K. Asai, J. Zhang,
T. Yanagida, S. Kasap
Presiding: K. Asai
- Poster Session**
19:00 – 21:00
- 2161.** New dosimetry technique using TL phosphor BeO:Na. **K. SHINSHO***, K. Otsubo, Y. Koba, G. Wakabayashi

- 2162.** Radiophotoluminescence response in Ag-doped phosphate glass irradiated with heavy particles.
H. Nanto*, T. Ikeguchi, Y.m. Yanagida, K. Hirasawa, Y. Takei, S. Kodaira, T. Yanagida, Y. Fujimoto, T. Kurobori, T. Yamamoto
- 2163.** Sm-doped fluorochlorozirconate (FCZ) glasses and glass-ceramics for scintillator applications.
G. Okada*, A. Edgar, S. Kasap, T. Yanagida
- 2164.** Scintillation and optically stimulated luminescence of ZnO -precipitated glass-ceramics.
H. Masai, T. Yanagida, T. Fujiwara
- 2165.** Luminescence property of MO_x -codoped with zincphosphate glasses.
H. Masai, T. Yanagida, Y. Fujimoto, M. Koshimizu
- 2166.** Scintillation responses of undoped CdF crystal.
T. Yanagida*, M. Koshimizu, Y. Fujimoto, G. Okada, K. Fukuda
- 2167.** Evaluation of undoped CdS semiconductor crystalline scintillator.
T. Yanagida*, M. Koshimizu, G. Okada
- 2168.** Comparative study of undoped and Eu-doped SrI₂ crystal scintillator.
T. Yanagida*, M. Koshimizu, G. Okada, T. Kojima, J. Osada
- 2169.** Spiropyran-based X-ray sensitive fiber.
K. Kinashi*, Y. Miyamae , R. Nakamura, W. Sakai, N. Tsutsumi

Saturday Morning

Hawaii Convention Center
317A

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

- Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: K. Akiyoshi, M. Tabrizian
- 8:00 – 2170.** Molecularly imprinted nanogels for human serum albumin recognition.
Y. Kitayama, R. SASAO, T. Takeuchi*
- 8:15 – 2171.** Phenylboronic acid-bearing nanoparticles as a versatile platform for preparing drug-conjugated nanoparticles using the Suzuki reaction.
A.J. van der Vlies, U. Hasegawa
- 8:30 – 2172.** Transdermal protein delivery systems controlled by photothermal effect of gold nanorods.
T. Niidome*
- 8:55 – 2173.** Enhancement of DNA enzyme activity by nano-assembling with cationic copolymers.
A. Maruyama, J. Gao, N. Shimada
- 9:20 – 2174.** DNA-assembled nanosystems for in vivo targeting.
W.C. Chan*
- 9:45** Intermission
- 10:00 – 2175.** Surface-enhanced Raman scattering nanoparticles for the detection and mapping of cardiovascular inflammatory biomarkers. K. Bowey, J. Tanguay, M. Sandros, **M. Tabrizian***
- 10:25 – 2176.** pH- and temperature-responsive organic-inorganic hybrid polymer nanoparticles with controlled cellular uptake.
Y. Hiruta*, S. Koide, J. Wang, H. Kanazawa
- 10:40 – 2177.** Effect of “reversely arranged” zwitterionic amphiphiles on protecting structure of liposomes during freeze-dry and rehydration.
T. Aikawa, Y. Takahashi, H. Okado, T. Kondo, M. Yuasa
- 10:55 – 2178.** Synthesis of protein-imprinted core/shell polymer particles bearing ON/OFF switchable molecular recognition property via CO₂/N₂ bubbling.
M. Isomura*, Y. Kitayama, T. Takeuchi
- 11:10 – 2179.** Polymer nanocomposites - an NMR investigation.
U. Scheler*
- 11:25 – 2180.** Size-selective polymer nanocapsules as a platform for yolk-shell hybrid nanocomposites.
S. Shmakov*, Y. Jia, E. Pinkhassik

Hawaii Convention Center
316A

Chemistry and Applications of Graphene (#39)

- Organized by: Y. Chen, R. Haddon, K. Loh
Presiding: Y. Huang, Y. Lee, Z. Liu, K.P. Loh

- 8:00 – 2181.** Chemically functionalized graphene for high performance electrochemical energy storage.
Y. Zhang
- 8:20 – 2182.** Growing high-quality graphene on insulators.
Z. Liu

- 8:40 – 2183.** Graphene molecules: Synthesis, electronic properties, and applications.
Z. Ji, **M. Sykora***

- 8:55 – 2184.** Intelligent polymer materials based on graphene.
Y. Huang*, Y. Zhang, J. Liang, L. Huang, Y. Chen*

- 9:10 – 2185.** Graphene oxide as a super material.
S. Hayami*, H. Takehira, K. Wakata, Y. Murashima

9:25 Break

- 9:45 – 2186.** Centimeter-scale monocrystalline graphene growth.
Y. Lee

- 10:05 – 2187.** CVD growth of 3D sp² structures and its application.
F. Wei*

- 10:25 – 2188.** Recent development in CVD graphene growth: Large area wafer scale growth and oriented grains.
K.P. Loh

- 10:45 – 2189.** Graphene electrodes for bio/chemical sensors.
A. Mulchandani*, R. Paul, S. Badhulika, R. Rajesh, P. Hammani, I. Terse-Thakoor, N.M. Saucedo, T. Tran, C. Villareal

- 11:00 – 2190.** 3D graphene and boron nitride nanosheets grown by chemical blowing.
X. Wang*
- 11:15 – 2191.** Peeling process of thin-film solar cells using graphene electrodes.
R. Ishikawa, S. Miyajima, M. Konagai

Hawaii Convention Center
321A

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

- Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie
Presiding: C. Bo

- 8:00 – 2192.** Oxygen-isotope exchanges in nanometer-sized ions as a window into geochemical processes.
W.H. Casey*

- 8:25 – 2193.** Chemistry of tetravalent actinide (U and Th) carboxylates: Isolation of oxo/hydroxo polynuclear clusters.
C. Faïsse*, C. Volkringer, C. hennig, T. Loiseau

- 8:45 – 2194.** Lanthanide “BottleBrush” clusters.
M. Massi*, M.I. Ogden, D. D’Alessio, R. Phe

- 9:05 – 2195.** Designer polyoxometalate – silver alkyne chimera cluster.
T. Ozeki*, M. Kurasawa, F. Arisaka

9:25 Flash posters

- 9:35 – 2196.** Structures and properties of uranyl peroxide cage clusters.
P.C. Burns

- 10:00 – 2197.** Structural variations in Group 13 heteropolyacids.
T.Z. Forbes, S.E. Mason

- 10:20 – 2198.** Group 13 (²⁷Al, ⁷¹Ga) studies of metal-oxide clusters.
B.A. Hammann, Z.L. Ma, K.M. Wentz,

- 10:35 – 2199.** Novel hybrid uranium-transition metal peroxide nanoclusters.
J. Qiu

- 10:50 – 2200.** Metal(IV)-oxide cluster formation: Understanding and controlling hydrolysis.
L. Soderholm*

- 11:15 – 2201.** Solid-state dynamics and hydrogen bonding in uranyl clusters using multinuclear MAS NMR spectroscopy.
T.M. Alam, M. Nyman, J. Yates

- 11:35 – 2202.** Main group coordination clusters: Synthesis, solution speciation, structure, and their use as “inks” for oxide materials.
D.W. Johnson

Hawaii Convention Center
321B

Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101)

- Organized by: F. Vetrone, S. Kohei, D. Ma, W. Huang, L. Huang, X. Peng

- 8:00 – 2203.** Growth of fluorescence-tunable gold clusters.
D. Mishra, F. Aldeek, G. Palui, **H. Mattoossi***

- 8:40 – 2204.** Surface plasmon enhanced photoluminescence of silver nanoparticles.
A. Pinchuk*, V. Kravets, K. Jiang

- 9:00 – 2205.** Correlating nanoparticle surface chemistry and photoluminescence via NMR spectroscopy.
J.E. Millstone

- 9:20 – 2206.** Ultrabright luminescence from gold nanoclusters.
D. Lee*

- 9:40 – 2207.** Development of bioluminescent sensor for rapidly detecting thrombin.
J. Zhang*

- 10:20 – 2208.** Protein protected luminescent gold nanoclusters and nanoparticles: Synthesis and their applications.
S. Yarramala, P. Chebrolu*

- 10:40 – 2209.** Surface functionalization of silicon nanocrystals for sensing platforms.
C.M. Gonzalez, Z. Yang, T.K. Purkait, M. Iqbal, S. Nesdoly, J. Veinot

- 11:00 – 2210.** Long-lived luminescent silicon nanoparticles for time-gated imaging.
J. Joo, X. Liu, E. Ruoslahti, M.J. Sailor*

- 11:20 – 2211.** Lanthanide complex based luminescent nanointerface: A versatile platform for molecular information conversion.
J. Liu*, H. Lei*

- 11:40 – 2212.** Near-Infrared (NIR) nanomaterials for bioanalysis.
F. Zhang

Hawaii Convention Center
319B

Development of Nano Devices and Nanotechnologies for Environmental Monitoring and Remediation (#124)

- Organized by: S. Al-Abed, D. Dionysiou, H. Choi, A. Bezbarua, J. Gardea-Torresdey, W. Choi, M. Litter, T. Lim, B. Pan
Presiding: S. Al-Abed

8:00 Introductory Remarks

- 8:05 – 2213.** Nanomachine-based accelerated environmental remediation.
J. wang

- 8:25 – 2214.** Sol-gel synthesis of metal-ion-modified TiO₂ photocatalysts for degradation of chlorinated organic compounds under visible light irradiation.

- S. Yamazaki***, N. Nishiyama, K. Tashiro, K. Adachi

- 8:45 – 2215.** Synthesis of Mg(OH)₂-coated nanoscale zero-valent iron (NZVI) for improved physical and chemical stabilities in environmental remediation.
Y. Hu*, X. Li*

- 9:05 – 2216.** Encapsulation of iron oxide nanoparticles and microorganism with extracellular polymeric substances: Envioning coupled adsorption-bioremediation of resistant pharmaceuticals.
H. Ha, S. Yoon, B. Mahanty, R. Kumar, S. Sen, C. Kim*

- 9:25 – 2217.** Synthesis of manganese oxide-coated magnetic nanoparticles and their catalytic efficiency for the oxidative degradation of bisphenol A.
A. Omoike*, K.N. Hall

* Principle Author

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<http://pacifichem.org/onlineprogram>

9:45 Break
9:55 – 2218. Inorganic oxyanion activation strategies using nanoscale materials: Application for oxidative degradation of organic pollutants. **J. Lee***, H. Yoo, Y. Ahn, E. Yun

10:15 – 2219. TiO₂ nanotube as deactivation-resistant photocatalyst for the removal of volatile organic compounds. **W. Choi***, S. Weon

10:35 – 2220. Photocatalytic degradation of contaminants of emerging concern using solar-visible light-active TiO₂. C. Han, **D. Dionysiou***

10:55 – 2221. Adsorption of CH₄ and N₂O from livestock using ZIF-8. **B. Delgado***, A. Avalos Ramirez, R. Lagace, S. Godbout, A. Giroir-Fendler

Hawaii Convention Center
320 Theatre

Functional Molecular Materials and Devices (#128)

Organized by: R. Kato, H. Mori, J. Schlueter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya
Presiding: H. Mori, B. Powell

8:00 – 2222. Magnetism and conductivity in triangular-lattice ET compounds under controlled randomness and doping. M. Urai, T. Furukawa, K. Miyagawa, H. Taniguchi, H. Oike, T. Sasaki, **K. Kanoda***

8:25 – 2223. Organic superconductors and quantum spin liquid candidates based on dimer-type ET materials κ -(ET)₂X. **G. Saito***, T. Hiramatsu, Y. Yoshida, A. Otsuka, M. Maesato, Y. Shimizu, H. Ito, H. Kishida

8:50 – 2224. Charge carrier injection into spin-liquid BEDT-TTF Mott insulators using ionic-liquid-gated transistors. **H. Ito***, K. Sato, Y. Era, S. Iguchi, S. Kurada, T. Hiramatsu, Y. Yoshida, G. Saito

9:10 – 2225. High pressure and high magnetic-field studies of the spin gapped organic Mott insulator with distorted triangular lattice. **M. Maesato***, Y. Yoshida, Y. Shimizu, T. Hiramatsu, G. Saito, H. Kitagawa

9:30 – 2226. Dual-functional molecular crystal. **B. Zhang***, D. Zhu

9:50 break

10:05 – 2227. Critically dielectric. **C. Hotta**

10:30 – 2228. Prediction of a spin-liquid ground state in the geometrically frustrated molecular crystal Mo₃S₇(dmft)₃. A.C. Jacko, C. Janani, H. Nourse, J. Merino, I. McCulloch, **B. Powell**

10:55 – 2229. Multi-band molecular conductors. **R. Kato***, T. Tsumuraya, T. Miyazaki, H. CUI

11:20 – 2230. Thermodynamic properties of spin liquid in dimer-Mott organic compounds. Y. Nakazawa, **S. Yamashita**, H. Akutsu, H. CUI, K. Ueda, H.M. Yamamoto, R. Kato

11:40 – 2231. Controlling crystallographic and electronic structure in completely organic cation radical salts. **J. Schlueter***

Hawaii Convention Center
315

Carbon Nanotubes: Preparation, Characterization and Applications (#227)

Organized by: S. Maruyama, R. Weissman, J. Liu, Y. Lee, J. Zhang
Presiding: S. Maruyama, J. ZHANG

8:00 – 2232. Tip enhanced Raman spectroscopy of carbon nanotubes. **R. Saito***

8:30 – 2233. Metrology of nanotube metallicity, its evolution, and the range of the Kataura plot. **P. Finnie***

9:00 – 2234. Emergent optical phenomena in carbon nanotubes. **Y. Miyachi***

9:30 – 2235. Asymmetry in resonant Raman excitation profiles of carbon nanotubes: The role of state-mixing. **E.H. Hároz***, H. Telg, E.B. Barros, J.A. Fagan, G. Ao, M. Zheng, J. Blackburn, **S.K. Doorn**

9:50 break

10:10 – 2236. Photon statistics and materials development towards single-photon emitters based on doped single-wall carbon nanotubes. **S.K. Doorn***, X. Ma, N.F. Hartmann, S. Yalcin, H. Htoon

10:40 – 2237. Optics and photonics with macroscopically aligned carbon nanotubes. **J. Kono***

11:10 – 2238. Preparation, measurement, and fractionation of monodisperse single wall carbon nanotubes. **P.J. Wyatt***

11:30 – 2239. Variance spectroscopy of single-walled carbon nanotube samples. **R. Weissman***, J. Streit, S. Bachilo, S. Sanchez

Hawaii Convention Center
318A

Advances in Bioinspired and Biomedical Materials (#245)

Organized by: K. Healy, Y. Ito, P. Messersmith, X. Chen, I. Kang
Presiding: I. Kang

8:00 Introduction

8:05 – 2240. Biomimetic water and oil selective open capillary prepared by surface modification. **S. Ito**, D. Ishii

8:25 – 2241. Evaluation of water evaporation suppression effect of plasma polymerized thin film of amphiphilic molecules. **H. Shibaaki**, D. Ishii, R. Kawamura

8:45 – 2242. Slippery interfaces: A new concept in antibiofouling materials. **J. Aizenberg***, C. Howell, S. Sunny

9:25 – 2243. Infrared invisibility stickers inspired by cephalopods. **L. Phan**, D.D. Ordinario, E. Karshalev, W.G. Walkup IV, **A.A. Gorodetsky***

9:45 – 2244. Construction and functionalization of regularly assembled structures composed of liquid crystalline filamentous viruses. **T. Sawada**, T. Serizawa*

10:05 Coffee Break

10:20 – 2245. Mechanically adaptive nanocomposites for biomedical applications. **C. Weder**

11:00 – 2246. Miniemulsion techniques to generate hollow capsules based on the dopamine self-polymerization: Tailoring the capsule shell chemistry, surface functionality, and applications. **A.M. Granville***, P. Zettler-Binnewies*, M. Stenzel, Y. Zhai, K. Fan

11:20 – 2247. Rigid and anisotropic coiled-coil proteins exhibit superior cell-penetrating activity. N. Nakayama, K. Hagiwara, Y. Ito, K. Ijiri, Y. Osada, **K. Sano***

Hawaii Convention Center
317B

Challenge for Rare Element-free Functional Materials (#291)

Organized by: H. Hosono, D. Ginley, Y. Lee

Presiding: H. Hosono

8:00 – 2248. Ubiquitous element strategy in materials research. **H. Hosono***

8:20 – 2249. Toward a sustainable society. **S. Murai***

8:40 – 2250. Achieving high thermoelectric performance in skutterudites without rare elements. **J. Snyder**

9:10 – 2251. Sustainable chalcogenide nanomaterials for thermoelectrics.

D. Mott*, M.S. Singh, K. Gupta, M. Koyano, S. Maenosono

9:30 – 2252. Development of novel quasi-solid electrolytes composed of lithium, sodium, or magnesium salts and small amount of organic solvent. **M. Moriya***, S. Nabeno, Y. Hanawa, W. Sakamoto, T. Yogo

9:50 Break

10:00 – 2253. Oxide artificial atoms. **N. Satoh***

10:20 – 2254. Thin films of electronic-spin delocalized neutral radical: Morphology and photoelectronic properties. T. Miyata*, **R. Tsuji**, M. Keishima, Y. Morita

9:40 Coffee break

10:40 – 2255. Carbon-centered neutral radicals/carbon nanotube composite cathodes for high-performance Li-ion rechargeable batteries. **R. Tsuji***, M. Fujisaki, H. Nobukuni, Y. Morita

11:00 – 2256. Transparent electrochromic transistor. M. Hirota, T. Katase, **H. Ohta***

11:20 – 2257. Intermetallic compounds of naturally-abundant transition-metal elements rival precious-group metals in the catalytic remediation of automobile exhaust. **H. Abe***, T. Tanabe, T. Fujita

11:40 – 2258. Earth-abundant nanoporous metal catalysts for exhaust-gas transformation. **T. Fujita***

Hawaii Convention Center
318B

Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials (#309)

Organized by: A. Smirnov, S. Bottle, R. Tamura
Presiding: S.E. Bottle, M.V. Fedin

8:00 – 2259. pH-Switching of nitroxide radical stability and orbital conversion. **M.L. Coote***, G. Grynnova

8:30 – 2260. Light sensitive alkoxyamines: New efficient agents for nitroxide mediated photopolymerization (NMP²). **J.P. Blinco**, E. Simpson, S. Bottle, D. Gigmes, J. Clement, Y. Guillaneuf

9:00 – 2261. Light-sensitive alkoxyamines as versatile spatially- and temporally-controlled precursors of alkyl radicals and nitroxides. M. Baron, J. Lalevée, O. Soppera, D. Gigmes, **Y. Guillaneuf**

9:20 Break

9:30 – 2262. Conjugation and bioconjugation from α -functional polymers obtained by nitroxide-mediated polymerization (NMP) initiated by N-hydroxysuccinimidyl- or az-lactone-functionalized alkoxyamines. V. DELPLACE, S. Harrisson, Y. Guillaneuf, S. Pascual, L. Fontaine, **J. NICOLAS***

9:50 – 2263. Radical-triplet pair interactions as probes of long-range polymer motion in solution. **M. Forbes**

10:10 – 2264. Inhomogeneity of intermolecular magnetic interactions in liquid crystalline phases of nitroxide radicals. **Y. Uchida**

10:40 – 2265. Preparation and magnetic properties of nitroxide radical liquid crystalline gels. **Y. Takenoto***, Y. Uchida, K. Suzuki, S. Shimono, T. Kato, J. Yamauchi, R. Tamura

11:00 – 2266. Further development of nitroxide spin probe technique for comprehensive determination of structural and dynamic characteristics of ordered soft media. **A.K. Vorobiev***, D. Pomogailo, N. Chumakova

Hawaii Convention Center
314

Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei, A. Wee, W. Chen, P. Weiss
Presiding: A.T. Wee

8:00 – 2267. Selective C–H activation and C–C coupling on metal surfaces. Q. Li, H. Zhang, B. Yang, K. Sun, **L. Chi**

8:30 – 2268. On-surface polymerization – a versatile synthetic route to novel 2D organic materials. **M. Lackinger**

9:00 – 2269. Bromine-functionalized pyrene derivatives on Au(111): self-assembly and on-surface polymerization. **B.V. Tran**, T. Pham, F. Song, M. Nguyen, M. Kivala, L. Gade, M. Stoehr

9:20 – 2270. Molecular-assembly mechanism enables simultaneous fabrication and connection of (3,1)-chiral-edge graphene nanoribbons. **P. Han***, K. Akagi, F. Federici Canova, H. Mutoh, S. Shiraki, K. Iwaya, P.S. Weiss, N. Asao, T. Hitosugi

9:40 Coffee break

9:55 – 2271. Comparative study of two perylene derivatives on Cu(111): Insight into the bonding mechanism.

M. Enache*, M. Matena, J. Björk, J. Lobo-Checa, T. Jung, M. Persson, L. Gade, M. Stöhr

10:15 – 2272. Covalent modification of graphite and graphite using diazonium chemistry: Tunable grafting and nanomanipulation. **J. Greenwood***, S. De Feyter*

10:35 – 2273. Photoresponsive supramolecular assemblies composed of photochromic diarylethenes: Investigation of concentration dependence of surface coverage at a liquid/solid interface using a nucleation-growth model. **T. Hirose**, S. Yokoyama, D. Frath, T. Sakano, K. Matsuda*

10:55 – 2274. Thermodynamic self-assembly of 2D/3D nanoarchitectures constructed on solid/liquid interfaces. **M. Kuniate***
11:25 – 2275. Patternning and cross-linking of self-assembled monolayers. **M.B. Zimmt***, Y. Yang, J. He, C. Fang, R. Shelp

Hawaii Convention Center
316C

Fundamentals and Applications of Nanomaterials for Energy Technologies (#348)

Organized by: S. Jin, G. Yu, T. Minegishi, S. Maldonado, J. He
Presiding: S. Maldonado, T. Wu

8:00 – 2276. On the effect of thiol-capped Au-NPs into molecular photovoltaic devices: Functionalization, size, and positional effects. C. Sartorio, S. Cataldo, S. Scaramuzza, V. Amendola, B. Pignataro

8:15 – 2277. Solar energy conversion via block copolymer nanostructure. **S. SUN***, T. Nguyen, M. Hasib, D. Wang

8:30 – 2278. Drastic enhancement of miscibility in p/n blends with liquid crystalline semiconductors toward organic photovoltaics. L. Sosa-Vargas, Y. Higuchi, T. Nakao, D. Okuda, A. Fujii, M. Ozaki, Y. Shimizu*

8:45 – 2279. From 3D to 1D nanostructured $\text{CH}_3\text{NH}_3\text{PbI}_3$ for high efficiency perovskite solar cells. **N. Park**

9:15 – 2280. Nano oxides for hybrid perovskite photovoltaic and nonvolatile memory applications. **T. Wu***

9:45 break

10:00 – 2281. Size-controlled synthesis of $\sim \text{ZnS}-\text{AgInS}_2$ solid solution nanoparticles and their visible-light-driven photocatalytic activity. **T. Torimoto***, Y. Kamiya, T. Kameyama, S. Kubawata

10:30 – 2282. Prolonged hot electron dynamics in plasmonic metal-semiconductor ($\text{Au}-\text{TiO}_2$) heterostructures with implications for solar photocatalysis. **W. Wei**

11:00 – 2283. Basic study to synthesize binary, ternary, and quaternary tin sulfide semiconductor nanoparticles in aqueous solution. **T. Mabuchi***, S. Yokoyama, H. Takahashi, K. Tohji

11:15 – 2284. Low-temperature solution deposition of nanostructured antimony sulfide and selenide thin films for photovoltaics. **C.L. McCarthy***, R. Brutney

* Principle Author

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11:30 – 2285. Effect of particle size of $\text{La}_5\text{Ti}_2\text{CuS}_5\text{O}_7$ on the photoelectrochemical properties. **J. LIU**, T. Hisatomi, G. Ma, T. Minegishi, Y. MORIYA, M. Katayama, J. Kubota, K. Domen*

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316B

Multi-scale & Synergistic Supramolecular Systems in Material and Biomedical Sciences (#357)

Organized by: S. Aoki, H. Chiu, K. Soga, N. Gianneschi, X. Bengang
Presiding: N. Gianneschi, B. XING

8:00 – 2286. Materials and system developments for OTN-NIR fluorescence bioimaging. **K. Soga**

8:25 – 2287. Using tumortropic monocytes to deliver magnetic nanoparticle/chlorin e6-encapsulated oxygen microbubbles to tumor hypoxia for improved efficacy of the combined hyperthermia and photodynamic therapy. **H. Chiu***, W. Huang, P. Wu

8:50 – 2288. NIR light mediated lanthanide upconversion platforms for biomedical imaging: How far can they go?. **B. XING***, X. Ai, J. Aw, F. Liu

9:15 – 2289. 3D printed bionic nanomaterials. **M. McAlpine**

9:35 – 2290. Development of aquacatalytic systems based on self-assembly of amphiphilic palladium NNC-pincer complexes and their application to the C-C bond forming reactions in water. **G. Hamasaka**, F. Sakurai, Y. Uozumi*

9:55 Break

10:00 – 2291. Biomimetic communication between functional molecules via photo-controlled ions in polymeric nanodomains. R. Bofinger, J. Thevenot, S. Lecommandoux, R. Oda, **N.D. McClenaghan***

10:20 – 2292. Two different mechanisms in highly efficient chromatographic separation of cyclic porphyrin trimers by use of modified silica-gel columns. **A. Satake***, A. Asaihi, K. Shirai

10:40 – 2293. Hierarchical and dynamic supramolecular systems. **S. Stupp***

11:05 – 2294. Liposomal spherical nucleic acids: A new approach to immunomodulatory therapies. **C.A. Mirkin***

Hawaii Convention Center
319A

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

Organized by: Z. Ye, C. Brown, T. Kiguchi
Presiding: P. Janolin

8:00 – 2295. Incipient relaxor KLT: Anomalous relaxation and phonon lifetimes. **P.M. Gehring***, C. Stock, G. Xu, D. Lamago, D. Reznik, M. Russina, J. Wen, L. Boatner

8:25 – 2296. Slow localized mode in the polar cluster of relaxor ferroelectrics near morphotropic phase boundary. **M. Matsuura**, G. Xu, Z. Xu, P.M. Gehring, H. Endo, K. Shibata

8:50 – 2297. Elastic ionoc polarization scenario in the dipolar glass and relaxors. **J. Dec***, W. Kleemann, Z. Trybula, S. Miga

9:05 – 2298. Lead-free relaxor ferroelectrics for electrocaloric cooling. **G. Suchaneck***, G. Gerlach

9:20 – 2299. Heterogeneity and relaxors: A synchrotron X-ray scattering study. **K. OHWADA***

9:45 Break

10:00 – 2300. Nonequilibrium behavior of uniaxial relaxor ferroelectrics with tungsten bronze structure. **S. Kojima**, K. Matsumoto, J. Dec, W. Kleemann

10:25 – 2301. Phase transitions in relaxor ferroelectric materials with tungsten bronze type structures. **S. Schmid**, T.A. Whittle

10:40 – 2302. Nanodomain structure and properties of PZT single crystals as compared with relaxor ferroelectrics. **Z. Ye***, A. Bokov

11:05 – 2303. Polarization rotation and domain wall dynamics in PZT crystals. **A. Bokov***, S. Gorfrman, Y. Xie, A. Davtyan, N. Zhang, A. Zozulya, M. Sprung, U. Pietsch, C. Gutt, Z. Ye

11:20 – 2304. Comparison of the neutron diffract scattering from PMN-PT and PZT. M. Krogstad, P.M. Gehring, S. Rosenkranz, F. Ye, Z. Ye, **D. Phelan**

11:35 – 2305. Structure and lattice dynamics of PZT crystals. **S. Vakhrushev***, D. Andronikova, Y. Bronwald, A. Bosak, D. Chernyshov, R. Burkovsky, I. Leontyev, Z. Ye

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322AB

Self-organization: Novel Mesogens and Applications (#447)

Organized by: H. Eichhorn, E. Choi, T. Hegmann, Y. Shimizu, K. Zhao
Presiding: H. Eichhorn

8:00 Opening Remarks

8:05 – 2306. Functionalization of polymerizable liquid crystalline semiconductors based on nanosegregation. **M. Funahashi***

8:35 – 2307. Playing with nanosegregation in discotic crown ethers: From molecular design to OFETs and nanofibers. **S. Laschat***

9:05 – 2308. Nanosegregated assembly of electron donor-acceptor binary discotic mesogens for organic electronics. **T. Sakurai***, Y. Tsutsui, S. Yoneda, S. Seki*

9:25 – 2309. Discotic dyads show segregated donor and acceptor superstructure and high charge carrier mobilities. **K. Zhao***, Y. Gao, L. An, W. Yu, J. Xu, Q. Zeng, H. Monobe, Y. Shimizu, B. Heinrich, B. Donnio

9:45 – 2310. Complex 3D architectures composed of discotic macromolecules. **T. Kajitani**, D. Hashizume, K. Motokawa, M. Takata, T. Fukushima*

10:10 – 2311. 2D and 3D self-organization of organic semiconductors. **E. Mena-Osteritz***, P. Bäuerle

10:40 – 2312. Liquid crystalline composites as organic semiconductors. K. Kawano, S. Nawamoto, H. Nishikawa, H. Monobe, Y. Shimizu*

11:00 – 2313. Hierarchical liquid crystalline structure in high proton conductive sulfonated polyimide films. **S. Nagano**, M. Hara, Y. Nagao

11:20 – 2314. Design and electrochemical transformation of redox-active metalomesogens. **H. Chang***

Hawaii Convention Center
Halls I, II, III

**Materials & Nanoscience General Posters
10:00 – 12:00**

Organic Materials

2315. Investigation of new chemical family of $n\text{-C}_x\text{H}_{(2x+1)}\text{N}(\text{Et}_2\text{Et}_3\text{Me})$ showing ionic plastic crystals ($x = 4-7$) and liquid crystals ($x = 8-18$). Y. Yamada, E. Kashimoto, S. Hirakawa, **H. Honda***

2316. Formation and reactivities of quinones derived from dopamine (DA) and 3,4-dihydroxy-phenylalanine (DOPA) derivatives: Versatile building blocks for functionalised materials?. S. Santhanakrishnan, W.Y. Cheah, C.L. Chai*

2317. Thermal properties of 2-bromo-5-chlorothiophene. **R. Kuwashima***, H. Fujimori, A. Nagoe, T. Sugimoto

2318. Thermodynamics of micellization of sodium dodecyl sulfate and dodecyl trimethyl ammonium bromide. **A. Solano-Domínguez***, D. Nivón-Ramírez, L. Reyes-García, R. Gómez-Balderas

2319. Favorable effects of superficially deacetylated chitin nanofibrils on the wound healing process. **R. Izumi**, K. Azuma, S. Ifuku

2320. Phase behavior and viscosity enhancement of nonamphiphilic fluorocarbon-hydrocarbon hybrid compounds in supercritical CO_2 . **Y. Sato**, S. Ogiwara, S. Ono, C. James, A. Yoshizawa, M. Sagisaka*

2321. Improved interface and CO_2 permeability by dual-functional amphiphilic PDMS-g-POEM comb copolymer micelles. **S. Kim***, J. Jung, J. Lee, C. Park, J. Kim*

2322. Thermal behavior of a liquid crystal, EBBA, confined within 1- and 3D pores. **N. Kinjo***, N. Kondo, T. Yoshimi, H. Fujimori

2323. Phase transition behaviors of liquid crystal, nCB, by DSC-Raman simultaneous measurements. **N. Kondo**, T. Yoshimi, H. Fujimori

Processing

2324. Stretching processing of hydroxyapatite/poly(ϵ -caprolactone) composite scaffolds. **K. Komatsu**, S. Umemoto, H. Minbu, T. Kawase, T. Tanaka*

2325. Preparation of photocatalytic thin films of tricalcium phosphate by doping $\text{Tl}^{(\text{IV})}$ and $\text{Zn}^{(\text{II})}$ ions. **N. Yoshida***, Y. Nakamura, T. Okura

2326. New preparation method of nanowires containing various organic molecules. **J. Nishijo***

2327. Preparation of hybrid films of layered silicon/germanium and organic material. **H. TACHIBANA***, R. AZUMI

2328. Photocatalytic degradation of bisphenol A in aqueous solution with modified ZnO . N. Hoshiyama, **H. Katsumata***, T. Suzuki, S. Kaneko

Electronic and Photonic Applications

2329. Net-patterned photocathode with Pt-sputtering for solid-state dye-sensitized solar cells with enhanced light reflection. **D. Kim***, C. Lee, J. Lim, D. Kim, J. Kim*

2330. Optical/electrical properties of electrochromic devices dependent on cell distance and electrolyte concentration. **C. Ah***, S. Cho, T. Kim, J. Song, H. Ryu, Y. Kim, H. Yu

2331. Conformation-insensitive ambipolar charge transport in a diketopyrrolopyrrole(DPP)-based co-polymer containing acetylene linkages. **H. Yun**, H. Choi, M. Kim, K. Cho, Y. Kim*, S. Kwon

2332. Novel class of organic semiconductors for solution processed organic electronics. **K. Park**, K. Cheon, Y. Lee, J. Lee, H. Song, D. Chung, S. Kwon, Y. Kim*

2333. Synthesis of phenanthro[1,10,9,8-cdef]carbazole-based conjugated polymers for organic solar cell applications. **J. Lee**, H. Yun, K. Park, E. AHN, Y. Kim*

2334. Comparative studies on the relations between composition ratio and charge transport of diketopyrrolopyrrole(DPP)-based random copolymers. **M. Sung**, H. Yun, K. Park, Y. Kim*, D. Chung

2335. Polymer nanolayer for advancing the electrical stability of OTFT. **C. Cho**, J. Baek, Y. Cheon, J. Lee, Y. Kim*

2336. Preparation of metal supported graphene substrate for STM. **H. Tanaka***, M. Taniguchi

2337. Fabrication of polypyrrole wrinkle topographies via a swelling-deswelling process for potential uses in tissue engineering. **J. Lee**, M. Aufan

2338. Tunable colloidal photonic crystals immobilized in soft hydrogels. **Y. Naoi**, T. Kanai*, T. Sawada

2339. Effect of different electron acceptors in carbazole-based double branched organic dyes on the performance of dye-sensitized solar cells. **J. Cho**, C. Son, S. Thogiti, D. Lee, J. Kim*

2340. Comparison of mono- and di-branched carbazole-based organic dyes for the p-type dye-sensitized solar cells. **N. Jung**, E. Kim, K. Ahn, J. Kim*

2341. Charge carrier mobilities in $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskites from first-principles calculation. **T. Zhao**, D. Wang, Z. Shuai

2342. Fabrication of organic fluorescent dye layered double hydroxide thin film on quartz crystal microbalance. **S. Aisawa***, M. Sawasato, J. Sang, H. Hirahara

2343. Novel UV protection agents based on optical stop band of colloidal photonic crystals. **T. Oki**, T. Kanai*

2344. Well defined conducting polymer (pedot/pss) microparticles. **S. Chuaychob**, P. Kanatharan, P. Thavarungkul, C. Thammakhet, M.W. Mak*

2345. Tubular solids of lanthanide-doped polyoxometalates in micrometer-scale: Synthesis and NIR-luminescent properties. **G. Li***, J. Peng*

2346. Graphene nanoribbon formed by templated sonochemistry. **S. Ju**

2347. Negative photoconductivity of graphen investigated by ultrabroadband optical pump terahertz probe spectroscopy. **M. Yamashita***, S. Keda, C. Otani

2348. Different structure ZnO particles enhanced the electrochemical property of graphene oxide by organic conjugation. **L.L. Zhong**

2349. Aggregation-induced emission (enhancement) and blue OLED application based on new oxazoline containing heteroleptic iridium(III) complexes. **W. Che***, D. Jin*, T. Yang*, **D. Zhu**, Z. Su

2350. Plasmonic properties of gold nano clusters assembled with thiol compounds. **N. Uehara***, C. Haneishi

2351. Synthesis of POSS-based aggregation induced fluorescent materials. **H. Zhou***

2352. Design and synthesis of a fluorescent chemosensor for the selective detection of heavy metal cations. **Y. Son**

2353. Synthesis of H^+ -conductive Narpsi glass-ceramics. **Y. Takahashi***, N. Yoshida, K. Yamashita, T. Okura

2354. Synthesis and evaluation of ionic conductivity of alkaline-doped Narpsi glass-ceramics. **Y. Ota**, N. Yoshida, K. Yamashita, T. Okura

2355. Electrical biosensor with nanomesh silicon channel via block copolymer lithography. **H. Jin**, C. Jeong, S. Kim*

2356. Optically switchable smart windows with integrated photovoltaic devices. **D. Ko**

2357. Synthesis and characterization of organic semiconductors on organic thin film transistors and organic photovoltaic cells. **M. Kim***, T. An*, H. Kim, M. Sung, C. Cho, J. Baek, K. Park, C. Park, Y. Kim*

2358. Conductive polymer composites with segregated structures. **H. Pang**, Z. Li*

2359. Development of dye-sensitized solar cell based on circularly arranged porphyrin array thin film. **S. Asaoka***, A. Kobayashi, Y. Tanio, T. Tokuoka, M. Aotani

2360. Phenothiazine-based multichromophoric organic dyes for dye-sensitized solar cell application. **Y. Lee**, S. Thogiti, Y. Han, J. Kim*

2361. Polymer with high hole mobility for efficient bulk heterojunction solar cells. **Y. Cheon***, X. Liu, S. Lee, Y. LEE, Y. Kim

2362. Nobel donor-acceptor type copolymer for solar cells. **H. Kim**, Y. Ha, S. Lee, Y. Kim*

2363. Crystalline properties and performances of devices are influenced by solvent boiling point. **S. Park**, E. AHN, Y. LEE, Y. Kim*

2364. Synthesis of bulk heterojunction for organic solar cell. **Y. Ha**, H. Kim, S. Lee, Y. Kim*

*** Principle Author**

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onlineprogram

- 2365.** In-situ electrical conductivity of Li_2MnO_2 nanowires as a function of "x" and size in energy storage device. **M. Le, R. Penner**
- 2366.** UV-irradiation treatment of photoelectrode for the flexible dye-sensitized solar cells. **T. Kim, B. Jang, S. Kim, J. Kim***
- 2367.** New ionic plastic crystals formed by cage type cations of 1-methyl-4-aza-1-azoniabicyclo[2.2.2]octane and 1-ethyl-4-aza-1-azoniabicyclo[2.2.2]octane with anions of BEt_3Me and BEt_4^- . **S. Hirakawa, Y. Kotani, H. Honda***
- 2368.** Preparation and characterization of photoresponsive p-n junction films. **K. Koga*, T. Suzuki**
- Organic Materials**
- 2369.** Hydrothermal growth of high crystalline CdS spheres with pebble surface. **N. Kim, H. MAENG, C. Ah, H. Yu**
- 2370.** Effect of different synthetic routes on the structural, morphological, and magnetic properties of Ce-doped LaFeO₃ nanoparticles. **b.s. randhawa***
- 2371.** Insight on superparamagnetic behavior of pure and Ag-doped zinc ferrite nanomaterials. **h. kaur***
- 2372.** Fabrication and properties of transparent functional silica glass using SiO_2/PVA mesoporous nanocomposite. **S. Fujino***
- 2373.** Borate based advanced materials. **D. Neiner*, L. Harrower, M.K. McCray, B. Yonke, D.M. Schubert**
- 2374.** Preparation of Mg-Al layered double hydroxide/hydroxyapatite nanocomposite and its sorption behavior with cadmium, lead and phosphate ions. **Y. Watanabe*, H. Yamada, K. Fujinaga, S. Oshima, Y. Komatsu**
- 2375.** Subsurface imaging of cobalt cores encapsulated within polystyrene nanoparticles using force modulation microscopy. **S.M. Deese, A.L. Francis, A.M. Taylor, J. Pyun, J.Y. Chan, J.C. Gamo**
- 2376.** Low-temperature formation of α -alumina from polyhydroxoauminum composite gels containing ascorbic acid and oxalic acid. **T. Yamaguchi, N. Mukouyama, S. Taruta**
- 2377.** Magnetoferent nanoparticles for targeting and visualizing tumor tissues. **L. Liang**
- 2378.** Synthesis and their properties of $\text{K}_2\text{SiF}_6\text{:Mn}^{4+}$ phosphors by coprecipitation method. **B. Bang, K. Choi, K. Choi, C. Kim***
- 2379.** Influence of the sintering density of Al_2TiO_5 by sintering method. **S. Yamagata, D. Yokota, A. Nagoe, T. Sugimoto, H. Fujimori**
- 2380.** Anisotropic growth-induced synthesis of dual-compartment Janus mesoporous silica nanoparticles for bimodal triggered drugs. **D. Zhao* Hybrid Materials**
- 2381.** Long-term stability of nanosilica/poly(ethylene glycol) reversible gel. **Y. Hirose**
- 2382.** Effect of metal substitution on the physical properties in the organic-inorganic hybrid tin iodide cubic perovskites. **K. Kobayashi, T. Inabe, J. Harada, Y. Takahashi, H. Hasegawa**
- 2383.** Influence of structural ordering on magnetic properties of iron oxide nanoparticles imbedded in a polymer matrix. **P. Daniel**
- 2384.** Fabrication of organic/inorganic composite micropatterns by anionic UV curing process. **A. Asai, M. Furutani, K. Arimitsu***
- 2385.** Characterization of spatially confined nanoclusters of porphyrines using conductive-probe atomic force microscopy. **X. Zhai, P. Derosa, J.C. Gamo**
- 2386.** Hydroxyapatite deposition on polyimide films containing carboxyl group in a biomimetic solution. **Y. Saegusa**
- 2387.** Fabrication process of covalently bonded CNT-on-CF composite fabrication of covalently bonded carbon nanotubes on carbon fibers and their application to nylon 6,6 composites. **J. Kim*, E. Choi, Y. Jo, c. kim**
- 2388.** Unique photoisomerization behavior of a dicationic azobenzene derivative adsorbed electrostatically at the two anionic sites on a clay nanosheet. **T. Shimada*, T. Umemoto, S. Takagi**

Self-assembled Structures

- 2389.** Protein- and carbohydrate-conjugated self-assembled nanodots for biological imaging applications. **S. Hsieh*, M. Kang, P. Lin**
- 2390.** Biomimetic peptide self-assembled nanostructure-Pd complex (PEP_{Pd}) cross coupling reactions in aqueous phase as recyclable catalyst. **S. Kim, N. Lee*, J. Ryu, S. Lee***
- 2391.** Preparation of cellulose nanofibers from watermelon peel and the composite with silver nanoparticle for endowing antifungal property. **R. Noda*, S. Ifuku**
- 2392.** Surface self-assembly of 4-(chloromethyl)phenyltrichlorosilane within exposed sites of Si(111) studied in toluene at selected temperatures. **P. Chambers, N. Kuruppu, J.C. Gamo**
- 2393.** Quantitative evaluation of sound-induced alignments of supramolecular nanofibers formed from perylenebisimide derivatives. **Y. Hotta, A. Tsuda**
- Applications**
- 2394.** Synthesis of new acrylamide-based block copolymers and their application to nanolithography. **Y. Han*, I. Byun**
- 2395.** Synthesis and properties of niobium borides by metal flux method. **s. okada*, y. takashi, y. kunio, s. toetsu, m. takao**
- 2396.** Water treatment using a wire mesh-supported TiO_2 photocatalyst. **K. Fujii*, T. Sugita, M. Mori, H. Itabashi**
- 2397.** Oxygen behavior during deoxidation of titanium powder using calcium deoxidizer. **J. Lim*, J. Oh, K. Roh, C. Sul**
- 2398.** Utilization of an anion-exchange type TiO_2 photocatalyst for water purification. **K. Kobayashi, T. Sugita, M. Mori, H. Itabashi**
- 2399.** Development of novel membrane materials using vertically aligned carbon nanotube for seawater desalination. **J. Jung, S. Lee, J. Sohn, J. Yoon**
- 2400.** UV and laser irradiation of functionalized gold nanoparticles as a potent antibacterial agent against the *Escherichia coli*. **S. godivardaraju**
- 2401.** Influence of halogen substitutions on rates of charge tunneling across SAM-based large-area junctions. **H. Yoon*, G. Kong, M. Kim**
- 2402.** Direct crosslink adhesion of polyamide and acrylonitrile butadiene rubber. **H. Hirahara, R. Sato, S. Aisawa, J. Sang**
- 2403.** Controlled release of antibiotics from etched titanium surfaces coated with hydroxyapatite microcapsules and polycaprolactone. **T. Shimada, Y. Nishino, I. Kimura, M. Taniguchi, T. Tanaka***
- 2404.** Synthesis of hollow nanosphere layered double hydroxide as cellular delivery vector. **S. Aisawa*, H. Takekura, J. Sang, H. Hirahara**
- 2405.** Adhesion of natural rubber and carbon steel plate. **H. Hirahara, K. Miura, S. Aisawa, J. Sang, J. Oravec**
- 2406.** Adsorption behavior of zearelenone by commercial and organophilic clays. **S. Aisawa, H. Yamazaki, J. Sang, S. Endo, M. Sekine, N. Takahashi, K. Sakao, E. Narita, H. Hirahara**
- 2407.** Synthesis and NO_x adsorption of MgO rich spinel Al_2MgO_4 powder by coprecipitation method. **s. okada*, y. takashi, y. kunio, s. toetsu**
- 2408.** Grafting of polyNIPAAm onto chitin nanofiber surface through atom transfer radical polymerization. **S. Tomiyama*, S. Ifuku**
- 2409.** Novel biological adhesives consists of carboxymethyl chitin derivative and chitin nanofiber. **J. Uchiyama*, M. Morimoto**
- 2410.** Structure of ice in poly-N,N,-dimethylacrylamide hydrogel. **Y. Takeuchi, Y. Sekine, T. Ikeda-Fukazawa**
- 2411.** Synergistic effects of bioinspired subnanoscale catalysts on the WO_3 nanofiber and their superior detection capability toward biomarker VOCs. **S. Kim***
- 2412.** Ozone nano-bubble water: Fundamental properties and washing effects. **Y. Yamaguchi*, Y. Nakamura**
- 2413.** Applications of nanodiamond composite materials. **T. Ogata*, S. Kim, T. Negi, K. Honda, S. Kurihara**
- 2414.** Improvement of contamination resistance of PET surface by atmospheric pressure plasma jet treatment. **K. Gotoh*, E. Shobuke, Y. Kobayashi**
- 2415.** Controlling of NBR surface chemical functional properties during the curing process. **J. Sang, S. Aisawa, H. Hirahara, K. Mori**
- 2416.** Development of novel DNA aptamers for the detection of circulating tumor cells using terahertz chemical microscopy. **E.M. Hassan, M.C. DeRosa*, W. Willmore, T. Ozaki**
- 2417.** Novel method to evaluate surfactant potency by TLC. **K. Chen, C. Indou, Y. Yamashita, K. Sakamoto**
- 2418.** Synthesis and Cs-adsorption behavior of phyllosilicates in saponite - phlogopite system. **H. Yamada, S. Yokoyama, Y. Watanabe, K. Morimoto, S. Suzuki, T. Yaita, T. Hatta**
- 2419.** Versatility of novel alkali metal chalcogenide ligands in colloidal nanoparticles. **S. Lee, S. Baek, S. Kim***
- 2420.** Specific solvent produces specific phase Ni nanoparticles: A pulsed laser ablation in solvents. **H. Jung*, M. Choi**
- 2421.** Synthesis and characterization of conjugated polymers for organic solar cell applications. **S. Lee, E. AHN, S. Park, Y. Kim***
- 2422.** Fabrication of monodisperse microbubbles using glass capillary microfluidic devices. **A. Matsuo, T. Kanai***
- 2423.** Preparations of cationic surfactant protected dendritic gold nanoparticles by tartaric acid reduction. **M. Takezaki, S. Shibata, K. Miyoshi, T. Tominaga**
- 2424.** Synthesis of multinuclear pt-thiolate complexes. **K. Ishihara, T. Imaoka, K. Yamamoto**
- 2425.** Solubilization of water in supercritical CO_2 by nonamphiphilic fluorocarbon-hydrocarbon hybrid compounds. **S. Ogiwara, S. Ono, Y. Sato, C. James, A. Yoshizawa, M. Sagisaka***
- 2426.** Silicon quantum dot porous nanocarrier for ultrasensitive high explosives detector. **J. Kim, H. Sohn***
- 2427.** Effect of halogen substitution on electronic properties in organometal halide hybrid perovskites. **H. Hasegawa*, Y. Takahashi, J. Harada, T. Inabe***
- 2428.** Study of adhesion between thermoplastic resin and metal using injection molding. **H. Hirahara, R. Kumagai, S. Aisawa, J. Sang**
- 2429.** Dynamic mechanical responses of interfacial water probed by amplitude-modulation atomic force microscopy. **T. Nyu, T. Hayashi***
- 2430.** Synthesis of carbon nanospheres/copper composite particles by electroless plating method. **S. Aisawa, T.T. Nguyen, H. Hirahara, J. Sang**
- 2431.** Adsorption behavior of silane coupling agent by the quartz crystal microbalance method and the nano thermal analysis. **H. Hirahara, S. Hiyama, S. Aisawa, J. Sang**
- 2432.** Mechanochemical synthesis of noble metal nanoparticles aided by $\text{P}(\text{IN}-\text{SiMe}_2)_3$. **N.C. Boyde, T.P. Hanusa***
- 2433.** Metal-substituted epsilon iron oxide nanoparticles exhibiting high-frequency electromagnetic wave absorption. **M. Yoshikiyo*, A. Namai, S. Ohkoshi**
- 2434.** Development of highly-efficient synthetic method of functional disulfide compounds and their applications to battery electrodes. **S. Balasubramanian, K. Ida, Y. Ishimizu, N. Tanifuji**
- 2435.** Atomization phenomenon of water with a surfactant. **H. Iwafuji*, A. Nagoe, T. Sugimoto, H. Fujimori, D. Yamada, S. Saisyo**
- 2436.** Thermal properties of benzene confined within mesoporous silica. **N. Tomita*, A. Nagoe, H. Fujimori**
- 2437.** Raman investigation on electric transport property of n-type 4H-SiC crystals co-doped with Al and N. **A. Minemura, T. Mitani, H. Fujimori**
- 2438.** Change of thermal expansion coefficient of $\text{Al}_{2-x}\text{Fe}_x\text{TiO}_5$. **T. Sugimoto, S. Yamagata, H. Fujimori**

- 2439.** Structures observation of titanate nanosheets, titanate nanotubes, and metal-doped nanotubes by HR-TEM. **T. Suzuki*, S. Okamoto**

- 2440.** Synthesis and characterization of perovskite photocatalyst. **K. Saito, T. Suzuki**

- 2441.** Switching behaviors of a porous alumina capacitor fabricated by anodization as a low temperature process. **K. Takase*, Y. Tanimoto, S. Otsuka, T. Shirimizu, S. Shingubara**

- 2442.** Mössbauer study of $\text{Sr}_3\text{Co}_2-x\text{Zn}_x\text{Fe}_{24}\text{O}_{41}$ Z-type hexaferite. **T. Kikuchi*, M. Kobune, M. Nakanishi, T. Fuji**

- 2443.** Synthesis of titanium dioxide nanotubular for advanced applications. **H. Bayraktar**

- 2444.** Preparation of core-shell microspheres with hybrid shell composed of multiple inorganic materials. **H. Yamamoto, N. Ryu, S. Nagaoka, M. Takafuji*, H. Ihara***

- 2445.** DSC and Raman spectroscopy simultaneous measurements of a liquid crystal, MBBA. **T. Yoshimi*, H. Fujimori, S. Hagiwara**

Saturday Afternoon

Hawaii Convention Center
317A

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: Z. Nie, J. Pyun

- 13:00 – 2446.** Materials synthesis in organic solvents: From metal oxide nanoparticles to films, aerogels, metallic foams, and organic/inorganic hybrids. **M. Niederberger***

- 13:25 – 2447.** Nanoparticle-stabilized nanocapsules for protein and nucleic acid delivery. **V.M. Rotello**

- 13:50 – 2448.** Synthesis and colloidal polymerization of inorganic nanoparticle monomers. **J. Pyun**

- 14:15 – 2449.** Directing the symmetry of stellated metal nanocrystals through seed selection. **S.E. Skrabalak**

- 14:40 – 2450.** Hybrid porous materials: Properties and applications. **L. De Cola, E.A. Prasetyanto, L. Maggini, I. Cabrera Puig**

- 15:05 Intermission**

- 15:20 – 2451.** In how far can we make nanoparticles mimic molecules?. **Z. Nie**

- 15:45 – 2452.** Self-assembly of complex terpolymer solution morphologies. **A.H. Mueller, T.I. Loebling, A.H. Groeschel, O. Ikkala**

- 16:10 – 2453.** Determination of the effective particle density of sterically-stabilised diblock copolymer nanoparticles. **S.P. Armes**

- 16:25 – 2454.** Functionalized BN materials and their potential applications. **Q. Weng*, Y. Bando, D. Golberg***

* Principle Author

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Hawaii Convention Center
316A

Chemistry and Applications of Graphene (#39)

Organized by: Y. Chen, R. Haddon, K. Loh
Presiding: X. Bao, Z. Bao, H. Cheng, P.V. Kamat

13:00 – 2455. Mass production of graphene and its application for anti-corrosion coatings. S. Pei, K. Huang, W. Ren, H. Cheng*
13:20 – 2456. Interface of graphene and organics. Z. Bao
13:40 – 2457. Copper- and Nickel decorated graphene as highly sensitive electrocatalysts for non-enzymatic oxidation of glucose for biosensor applications. D. Qazzazie*, M. Beckett, R. Mühlaupt, O. Yurchenko, G. Urban
13:55 – 2458. Degradation of aqueous glyphosate over graphene-based sunlight-driven photocatalyst. M. Feriani, K. Belkacemi, S. Hamoudi*

14:10 – 2459. Conduction limitations of fully reduced chemically converted graphene. S.V. Petersen*, B.W. Laursen, W. Hu
14:25 Break
14:45 – 2460. Cationic graphene-based nanohybrid for water purification. M. Chan-Park
15:05 – 2461. Catalysis over graphene and 2D materials. X. Bao*

15:25 – 2462. Efforts are underway to introduce luminescent quantum dots into the multifunctional catalyst mat and further enhance the capability of detection and removal of low concentrations of chemicals from water and air. P.V. Kamat*. R. Alam, V. Bridewell
15:45 – 2463. Reduced water vapor transmission rate of graphene gas barrier films for flexible organic field-effect transistors. K. Choi*, B. Hong
16:00 – 2464. Controlled growth of a graphene charge-trapping layer for organic nonvolatile memory transistors. S. Park*, Y. Park*, T. Choi, J. Seo
16:15 – 2465. Fe-catalyzed etching of graphene layers. G. Cheng*, I. Calizo, A. Hight Walker

Hawaii Convention Center
321A

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie
Presiding: G.R. Patzke

13:00 – 2466. Polyoxometalate assemblies and their elaboration. C. Ritchie*, M.R. Healey, H. Karoui
13:20 – 2467. Molecular cluster batteries of nano-hybrid materials between POMs and nanocarbons. K. Awaga*

13:40 – 2468. Electron transfer properties through monolayers of polyoxometalates covalently immobilized on electrodes. F. VOLATRON, C. RINFRAY, S. RENAUDINEAU, G. IZZET, A. PROUST*

14:05 – 2469. Magnetic POMs in molecular spintronics and quantum computing. E. Coronado, J. Baldoví, S. Cardona-Serra, A. Gaita, J. Clemente Juan

14:35 – 2470. Mixed-metal hybrid polyoxometalates with amino acid ligands: structural and electronic versatility.

C. Boskovic*, F. Akhlaghi Bagherjrei, M. Vonci, C. Ritchie, R. O'Hair, J. Zhang, G. Bryant, X. Lopez, J. Poblet

14:55 – 2471. Localized and delocalized excited states in Ti6 and Ti7 polyoxotitanate clusters. J. Bao, J. Benedict, J.R. Miller, P. Piotrowiak*

15:15 – 2472. Photoreduction process of nucleotide-coordinated polyoxomolybdates. E. Ishikawa*

15:30 Flash Posters

15:40 – 2473. Using Fourier transformed AC voltammetry to provide new insight into electrocatalysis with polyoxometalates. A.M. Bond*, J. Zhang, S. Guo, Y. Liu
16:05 – 2474. Redox-induced selective uptake-release of cations in porous ionic crystal based on polyoxomolybdates. S. Uchida*, R. Kawahara, S. Seino
16:25 – 2475. The iron Keggin ion from water. M. Nyman, O. Sadeghi
16:45 – 2476. Cation-induced conformational changes in uranyl-peroxide nano-clusters and their effect on anion molecular dynamics. M. Dembowksi, W.H. Casey, P.C. Burns

Hawaii Convention Center
321B

Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101)

Organized by: F. Vetrone, S. Kohei, D. Ma, W. Huang, L. Huang, X. Peng
13:00 – 2477. PEtOated silica nanocapsules via interfacial templating condensation for bioimaging. X. Li, Y. Zhang, S. Wong, Y. Chiang
13:40 – 2478. Synthesis of silica nanoparticles modified chemically with terbium complexes through Schiff base formation and their fluorescence properties in water. Y. Nakahara*, Y. Tatsumi, I. Akimoto, S. Osaki, M. Doi, K. Kimura
14:00 – 2479. Luminescent biohybrid nanomaterials from nanocellulose and carbon dots (CDs). J. Guo, K. Junka, E.I. Filippone*, J. Laine, O.J. Rojas
14:20 – 2480. Nanodiamond-based quantum biosensors. K. Briggman*, M. May
14:40 – 2481. Preparation of P-g-C₆N₄ nanodots and its fluorescence detection of Cu²⁺. X. Chen

15:00 – 2482. Drug release in polyester thin films: Release kinetics regulated by NIR stimulation through photoactive nanocomposite additives. T. Cheng*, F. Ortiz, R. Naccache, F. Vetrone, R.S. Marks, T.W. Steele

15:40 – 2483. Engineering of multicolor highly luminescent carbon nanodots for long-term bioimaging of plant cell physiological processes. L. Alexandre, R. Sekiya, M. Yoshikawa, Y. Moriyasu, S. Nakabayashi

16:00 – 2484. Nanophosphors as sensitive reporters in point-of-care diagnostics. A.S. Paterson, B. Raju, G. Garvey, A. Buell, K. Kourentzi, R.C. Willson*

16:20 – 2485. Luminесcent properties of europium-doped (H₂O)Y₃F₁₀ nanocrystals. A.M. Ritchie*, D. Boudreau, C. Caron, B. Richard

Hawaii Convention Center
319B

Development of Nano Devices and Nanotechnologies for Environmental Monitoring and Remediation (#124)

Organized by: S. Al-Abed, D. Dionysiou, H. Choi, A. Bezarbari, J. Gardea-Torresdey, W. Choi, M. Litter, T. Lim, B. Pan
Presiding: S. Al-Abed

13:00 – 2486. TiO₂ nanoparticles coated with polyoxometalate water oxidation catalysts: New systems for sustained light-induced water oxidation. S.M. Lauinger, J. Sumilner, Q. Yin, Z. Xu, E.N. Glass, T. Lian, C.L. Hill*

13:20 – 2487. Generation of reactive oxygen species on metal-doped SnO₂ electrocatalysts: Development, applications, and implication. H. Park*

13:40 – 2488. Monitoring of biological toxins in harmful algal blooms: From current approaches to future strategies. H. Choi*

14:00 – 2489. Degradation of cyanotoxins by ferrite-based nanomaterials. B. Ren, Y. Huang, C. Han, V. Sharma, K. O'Shea, D. Dionysiou*

14:20 Break

14:30 – 2490. Peptide array platform for detecting the presence of naphthenic acids in petroleum process affected water. S. Bhattacharjee, K. Kaur

14:50 – 2491. Interference lithography (IL) generated microarray as surface-enhanced Raman spectroscopy (SERS) substrates for pharmaceutical products in water detection. K. Hong, J. Menezes, A.G. Brolo*

15:10 – 2492. Femtomolar chemical detection on a metal-dielectric-CNT surface by surface enhanced Raman spectroscopy. H. Park, A.O. Altun

Hawaii Convention Center
320 Theatre

Functional Molecular Materials and Devices (#128)

Organized by: R. Kato, H. Mori, J. Schlueter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya
Presiding: C. Rovira, S. Uji

13:00 – 2493. Ferroelectricity in quasi-2D organic charge-transfer salts. M. Lang*

13:25 – 2494. Phase control and quantum critical behavior of ferroelectric charge-transfer complexes. S. Horuchi, K. Kobayashi, R. Kumai, F. Kagawa, Y. Tokura

13:50 – 2495. Fluorescent ferroelectrics of hydrogen-bonded alkylamide-substituted pyrene derivatives. T. Akutagawa*

14:15 – 2496. Noncovalent interactions in molecular quantum magnets. J.L. Manson*

14:35 – 2497. Spin crossover with thermal hysteresis (memory): The importance of scan rate and relaxation rate studies.

S. Brooker*, R. Kulmaczewski, J. Olgun, J. Kitchen, H. Feltham, R. Miller, G. Jameson, S. Narayanaswamy, J. Tallon
14:55 break

15:10 – 2498. Conductivity and magnetic ordering in multi-orbital radicals. R.T. Oakley*

15:35 – 2499. Controlled under pressure: Magnetic resonance studies of molecular materials. S. Hill*, K. Thirunavukkurasu, S. Winter, R.T. Oakley

16:00 – 2500. Designing of quantum spin magnets by π-conjugated organic radicals. Y. Hosokoshi*

16:20 – 2501. Light-induced radical trapping and large thermal hysteresis in magnetically bistable organic radicals. H. Phan, A. Dragulescu-Andrasi, K. Lekin, S. Winter, R.T. Oakley, M. Shatruck

Hawaii Convention Center
315

Carbon Nanotubes: Preparation, Characterization and Applications (#227)

Organized by: S. Maruyama, R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: Y. Lee, S. Maruyama

13:00 – 2502. Purification of horizontally aligned arrays of single walled carbon nanotubes. J. Rogers

13:30 – 2503. Exploring the growth of graphene and related 2D materials for electronic applications. H. Ago*

14:00 – 2504. Bio-electronics applications of carbon nanotube thin films. Y. Ohno

14:30 – 2505. Carbon nanotube electronics – more and more than Moore. L. Peng*, Z. Zhang, S. Wang, X. Liang

15:00 break

15:20 – 2506. Interaction of water molecules with single-walled carbon nanotube. Y. Homma, S. Chiashi, T. Yamamoto

15:50 – 2507. Carbon nanotube-based remarkably durable polymer electrolyte fuel cell. N. Nakashima*, I. Hafez, M. Berber, T. Fujigaya

16:20 – 2508. Floating catalyst CVD synthesis of SWNTs for thin film applications. E.I. Kauppinen*

14:20 Break

14:50 – 2521. Computational materials discovery. A.R. Oganov

15:20 – 2522. Thermodynamic and other related properties of titanium-dioxide systems. Y. Aoki*, S. Saito

Hawaii Convention Center
318A

Advances in Bioinspired and Biomedical Materials (#245)

Organized by: K. Healy, Y. Ito, P. Messersmith, X. Chen, I. Kang
Presiding: K. Healy

13:00 – 2509. Design, synthesis, and folding of sequence-defined peptoid polymers into bioinspired nanoarchitectures. R. Zuckermann

13:40 – 2510. Synthetic copolyamphophytes inspired by a mussel foot protein. S. Seo, S. Das, P. Zalicki, R. Mirshafiani, C. Eisenbach, J.N. Israelachvili, J. Waite, K. Ahn*

14:00 – 2511. Design of discrete DNA-modified gold nanoparticle assemblies with a beads-on-a-string-like structure and their interparticle distance changes depending on terminal base-pairing. Y. Akiyama, H. Shikagawa, N. Kanayama, T. Takarada*, M. Maeda
14:20 – 2512. Bioactive carriers for intracellular delivery of biologic and small molecule drugs. P. Stayton

15:00 Coffee Break

15:20 – 2513. Bioinspired encapsulation of Jurkat cell within titania artificial shell. E. Ko*, W. Youn, I. Choi*

15:40 – 2514. Comparison of cytokines secretions from macrophage cultured on hydroxyapatite and carbonated apatite dense ceramics. K. Igeta*, K. Nozaki, M. Aizawa, K. Yamashita, A. Nagai

16:00 – 2515. Microbial encapsulation in alginate/polydopamine core/shell microbes. B. Kim*, I. Choi*

16:20 – 2516. Alternative approaches for prevention of *Pseudomonas aeruginosa* biofilm formation on urinary catheters. T. Tzanov, M. Fernandes*, K. Ivanova, A. Francesko

Hawaii Convention Center
317B

Challenge for Rare Element-free Functional Materials (#291)

Organized by: H. Hosono, D. Ginley, Y. Lee

13:00 – 2517. Searching for rare element-free rare earth permanent magnets. m. sagawa

13:30 – 2518. Permanent magnets free from rare elements. K. Hono*

14:00 – 2519. Large perpendicular magnetic anisotropy in noble metal-free manganese nitride epitaxial thin film. A. Chikamatsu*, X. Shen, K. Shigematsu, Y. Hirose, T. Fukumura, T. Hasegawa

14:20 – 2520. Electrically controlled electromagnetic phase conversion in magnetic oxide at room temperature. T. Katase*, Y. Suzuki, H. Ohta*

14:40 Break

14:50 – 2521. Computational materials discovery. A.R. Oganov

15:20 – 2522. Thermodynamic and other related properties of titanium-dioxide systems. Y. Aoki*, S. Saito

* Principle Author

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TECHNICAL PROGRAM

15:40 – 2523. Computational crystal structure prediction of mixed valence tin oxide photocatalysts. **N. Umezawa**, J. Wang, H. Hosono

16:00 – 2524. Computational and experimental identification of earth-abundant ternary nitrides. Y. Hinuma, T. Hatakeyama, Y. Kumagai, Y. Muraba, H. Sato, H. Hiramatsu, I. Tanaka, H. Hosono, **F. Oba***

16:20 – 2525. On the existence and characterization of molecular electrode. **M. García Barrón***, V. Postils, M. Solà, J. Luis, E. Matito

16:40 – 2526. Structural and spectroscopic characteristics of C12A7 electrode glass: A DFT study. **L.E. Johnson***, P.V. Sushko, H. Hosono

Hawaii Convention Center
318B

Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials (#309)

Organized by: A. Smirnov, S. Bottle, R. Tamura
Presiding: K. OKADA, R. Tamura

13:00 – 2527. New aspects of nitronyl nitroxides in materials science. **K. OKADA**

13:30 – 2528. Nitroxide-copper clusters as building blocks for thermo/photoswitchable nanomaterials. **M.V. Fedin***

14:00 – 2529. Evaluation of β value of π -conjugated molecular wires by probing exchange interaction between two nitroxide radicals. **K. Matsuda***

14:30 – 2530. Control of phase transition behaviors of nitroxide radical paramagnetic liquid crystals. **T. Akita***, Y. Uchida, N. Nishiyama

14:50 Break

15:05 – 2531. Air-stable carbon-centered neutral radicals: Challenges for electrodeactive materials. **Y. Morita***, H. Nobukuni, T. Murata, M. Keishima, R. Tsuji

15:35 – 2532. Construction of molecular self-assemblies carrying a nitronyl nitroxide radical and effect of selective deuteration. **N. Yoshioka***, Y. Emura, T. Saito, N. Ozora, Y. Miura

16:05 – 2533. Adding redox-active nitroxides to the surface of carbon-based materials. **S.E. Bottle***, J.P. Blinco, A. O'Mullane, H. Zhu

16:35 – 2534. Spin probe and label studies of alumina-based functional materials and systems. **E.G. Kovaleva***, L.S. Molochnikov, L.F. Hatmullina, D.P. Stepanova, A. Smirnov, K.V. Kozhikhova, M.A. Mironov, A.V. Pestov

Hawaii Convention Center
314

Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei, A. Wee, W. Chen, P. Weiss

13:00 – 2535. Testing functional molecular assemblies by single-molecule manipulation. **L. Grill***

13:30 – 2536. Create and manipulate quantum states on surface using molecules. **N. Lin**

14:00 – 2537. Synchronization in self-assembled molecular machine networks. **S.W. Hla**

14:30 – 2538. Spin state of Iron phthalocyanine (FePc) on metal surfaces. **M. Kawai***, N. Tsukahara, N. Takagi

14:50 – 2539. Modulating charge transport mechanisms by tuning the architectures of supramolecular assemblies. A. Vilan, A. Pawlicki, B. Ewers, C. Drain, J. Batteas

15:10 Coffee break

15:20 – 2540. Electric-field-induced phase transformations at nanoscale. **O. Ivasenko**, Y. Fang, K. Cui, S. Lee, Z. Li, S. Mertens, S. De Feyter*

15:40 – 2541. Single molecule chemistry for surface assembly of DNA nanostructures. **T. Ye***, G.R. Abel, X. Hao

16:00 – 2542. Anthraquinone and pentaquinone pores on Cu(111): network formation through substrate electron confinement and its impact on guest dynamics. **L. Bartels**

16:30 – 2543. Design and manipulation of functional molecular nanosystems at interfaces. **J.V. Barth**

Hawaii Convention Center
316C

Fundamentals and Applications of Nanomaterials for Energy Technologies (#348)

Organized by: S. Jin, G. Yu, T. Minegishi, S. Maldonado, J. He
Presiding: S. Jin, W. Wei

13:00 – 2544. Water splitting on particulate and/or plate type photocatalysts. **K. Domen***

13:30 – 2545. Solar hydrogen production using carbon quantum dots and a molecular catalyst. **B. Martindale**, G. Hutton, C.A. Caputo, E. Reisner*

13:45 – 2546. Semiconductor nanowires for artificial photosynthesis of value-added chemicals. **P. Yang**

14:15 – 2547. Solar energy conversion and electrocatalysis using earth-abundant nanomaterials. **S. Jin**

14:30 break

14:50 – 2548. Graphene and C₃N₄-based electrocatalysts for energy conversion. **S. Qiao***

15:20 – 2549. Metal-free, heteroatom-doped carbon nanomaterials as sustainable electrocatalysts for fuel cells and water splitting. **T. Asefa***

15:35 – 2550. Electrochemical nanotechnologies: Batteries and electrocatalysts. **Y. Cui**

16:05 – 2551. Nanoparticle-assisted electrochemical synthesis of ammonia from water and nitrogen under atmospheric pressure. **K. Kim, H. Yoon*, J. Han***

16:20 – 2552. Block copolymer template-directed synthesis of mono- and bimetallic nanoparticle catalysts. **D. Rider**

Hawaii Convention Center
316B

Multi-scale & Synergistic Supramolecular Systems in Material and Biomedical Sciences (#357)

Organized by: S. Aoki, H. Chiu, K. Soga, N. Gianneschi, X. Bengang
Presiding: S. Aoki, H. Chiu

13:00 – 2553. Stimuli-responsive materials for biological and materials applications. **B.S. Sumnerlin**

13:25 – 2554. New approach for targeted assembly – copolymer blending vs. precision synthesis. **R.K. O'Reilly***

13:50 – 2555. De novo synthesis of artificial phospholipid membranes. **N.K. Devaraj**

14:10 – 2556. Transferring light energy into rotation of non-absorbing polymers through hydrogen and halogen bonds. **J. Vapaavuori**, I. Heikkilä, V. Dichiariante, G. Resnati, P. Metrangolo, R. Sabat, C. Bazzini, A. Primiggi, C. Pellerin

14:30 – 2557. Air-liquid interfacial self-assembly of conjugated block-copolymers into ordered nanowire arrays. **S. Park***, M.M. Cativo

14:50 Break

14:55 – 2558. Selective binding of guest alkyl termini by p-t-*butylcalix[5]arene* in the solid state. **R. Sekiya***, Y. Kajiki, T. Haino

15:15 – 2559. Assembly and application of Janus nanosheets. B. Rodier, P. Wei, Q. Luo, S. Burton, E. Mosher, **E. Pentzer**

15:35 – 2560. Self-assembled benzimidazolium salts and their strong antimicrobial properties. **C. Elie***, A.R. Schmitz

15:55 – 2561. Lanthanide-based nanoparticles as new candidates for nanothermometry. **E. Hemmer***, M. Quintanilla, F. Légaré, F. Vetrone

16:20 – 2562. Porphyrin supramolecular assembly: From nano to micro, and back. **G. Zheng**

Hawaii Convention Center
319A

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

Organized by: Z. Ye, C. Brown, T. Kiguchi
Presiding: P.M. Gehring

13:00 – 2563. Insights into the local structure of ferroelectrics via pair distribution function studies. **J.L. Jones***, T. Usher, I. Levin, E. Aksel, J. Forrester

13:25 – 2564. Understanding the morphotropic phase boundary in samarium-modified bismuth ferrite. **N. Valanoor***

13:50 – 2565. Defect induced phase states in perovskite nanoparticles. **I. Golovina***

14:05 – 2566. Correlation between antiferroelectric-like and ferroelectric components in the local region of polar materials. **Y. Liu**

14:25 Break

14:35 – 2567. Synthesis and characterization of (K, Na)NbO₃ Lead-free piezoelectric nanocrystals. **J. Li, L. Cheng, Y. Xu, K. Wang**

15:00 – 2568. One pot synthesis of nano ferroelectric materials by abnormally accelerated solid state reaction. **K. Toda**

15:20 – 2569. Development of ferroelectric oxides with oxygen tetrahedra. **H. Taniguchi***

15:45 – 2570. Functionality of dielectric/ferroelectric stacked layers. **C. Hwang***

16:10 – 2571. High piezoelectric properties of KNN-based piezoelectric ceramics: Preparation, characterization, and mechanism. **J. Zhu***, D. Xiao, J. Wu

Hawaii Convention Center
322AB

Self-organization: Novel Mesogens and Applications (#447)

Organized by: H. Eichhorn, E. Choi, T. Hegmann, Y. Shimizu, K. Zhao
Presiding: T. Hegmann

13:00 – 2572. Synthesis and self-assembly of novel dibenz[a,c]anthracenes: Influence of structure on mesomorphic properties. **K. Maly***, K. Psutka, J.A. Paquette

13:20 – 2573. Low symmetry triazine derivatives for crystal and liquid crystal engineering. **H. Taing, H. Eichhorn***

13:40 – 2574. Dynamically self-assembled nanoparticles as tunable metamaterials. **E. Gorecka***

14:10 – 2575. Liquid crystal directed nano-assemblies. **L.S. Hirst***

14:40 – 2576. Cholesteric liquid crystals: Polymer + nanoparticles. **T.J. Bunning***, I. de sia, N. Tabirian, S. Serak, T.J. White

15:00 – 2577. Enhancement of luminescence intensity in cholesteric liquid crystalline microcapsule. **Y. Iwai***, Y. Uchida, N. Nishiyama

15:20 – 2578. Porous biocompatible liquid crystal elastomer and their use as spatial cell culture scaffolds. **E. Hegmann***, R. Clements, E. Freeman, C. Malcuit, J. McDonough, L. Korley

15:40 – 2579. Design of novel amphiphilic mesogens and their complex mesophase morphologies. **X. Cheng**

16:10 – 2580. Patterning of mechanoinduced change in photoluminescent color on side chain liquid-crystalline polymer containing low molecular weight liquid-crystalline mechanochromic compound. **M. Kondo***, T. Nakaniishi, S. Miura, N. Kawatsuki

16:30 – 2581. Self-organized polymer patterns obtained on the periodically deformed liquid crystals as reaction media. **S. Kang***

Saturday Evening

Hawaii Convention Center
317A

Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)

Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: J. Texter

19:00 – 2582. Temperature-responsive properties of poly(*N*-isopropylacrylamide) nanoparticles bearing a peryleneimide group around the chain center. **S. Machida***, Y. Uchihashi, N. Ikeda

19:15 – 2583. Synthesis and assembly of hybrid anisotropic particles. **N. Wu**, S. Wang

19:30 – 2584. Synthesis of size-tunable polymeric nanoparticles by means of an elongational flow device and their incorporation in hybrid polymeric materials. **W. Yu, N. Visavelya, I.U. Khan**

C.A. Serra, M. Köhler, R. Müller, M. Bouquet, I. Kraus, S. Schmutz

19:45 – 2585. 2D ordered array of PEGylated ferritin. **M. Unema**, C. He, N. Okamoto, i. yamashita, Y. Uraoka

20:00 – 2586. New class of colloidal crystals. **J. Texter**

20:15 – 2587. Synthesis and functional evaluation of Eu-Mn complex nanoparticles for dual photoacoustic and magnetic resonance imaging probes. **Y. Kimura**, T. Kurimoto, Y. Imai, H. Imai, T. Matsuda, A. Toshimitsu, T. Kondo*

20:30 – 2588. Room temperature synthesis of graphene – Mn₃O₄ composite using different solvent system for supercapacitor application. **S. Syed Abdulrahim**, D. Sappani, V. THIRUMALAI, P. Balaya*, S. Valiyaveettil*

Hawaii Convention Center
321A

Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)

Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie
Presiding: M. Bonchio

19:00 – 2589. Self-assembly of polyoxometalates for flexible ionic organic frameworks. **L. Wu***

19:20 – 2590. Distortions in decavanadates and how that may impact interactions with biological interfaces. **I. Sanchez-Lombardo**, S. Alvarez, N. Levinger, **D.C. Crans***

19:40 – 2591. Polyoxometalates as a novel class of artificial proteases. **T.N. Parac-Vogt**, K. Stroobants, G. Absilis, H. Ly, A. Sap

20:10 – 2592. Recent developments in polyoxo-noble-metalate chemistry. **P. Yang**, Z. Lin, **U. Kortz***

20:30 – 2593. Understanding the assembly of gigantic polyoxometalate clusters with information theory and symmetry. **L. Cronin***

* Principle Author

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Hawaii Convention Center
Halls I, II, III

Development of Nano Devices and Nanotechnologies for Environmental Monitoring and Remediation (#124)

Organized by: S. Al-Abed, D. Dionysiou, H. Choi, A. Bezaruaah, J. Gardea-Torresdey, W. Choi, M. Litter, T. Lim, B. Pan

Poster Session
19:00 – 21:00

- 2594.** Application of nanosized ferric oxides-based adsorbent for phosphate removal and recovery from biotreated effluent. **Y. Zhang**, B. Pan*
- 2595.** Nanozerovalent iron: Preparation using natural antioxidants and reactivity toward the degradation of trichloroethylene. **J. Scott***, K.P. Weber, J. Ring, M. Chaung, K. Naylor
- 2596.** Atmospheric aerosol measurement using Recovery Sonde System. **Y. Park***
- 2597.** Colorimetric probe to determine Pb^{2+} using functionalized silver nanoparticles. K. Noh, Y. Nam, **K. Lee***
- 2598.** Removal of adhered uv-curable resin to the microstructure of mold by high hydrostatic pressure treatment. **T. Minamide**, A. Shimizu, U. Kajiwara
- 2599.** Resistive response of carbon nanotube membrane for the detection of chlorophenols. **W. Den**, E. Kanchanatip, N. Gridanurak
- 2600.** Colorimetric detection of zinc ion in aqueous solution using label-free silver nanoparticles. S. Lee, **Y. Nam**, K. Lee*
- 2601.** Cerium and lanthanum-modified, magnetically separable nanocatalysts for water treatment. C. Han, J. Lalley, X. Li, **M. Nadagouda***
- 2602.** Potential application of green nano- TiO_2 on the photocatalytic degradation of azo dyes present in tannery effluents: Effect of nanoparticle concentration and size. J. Ibarra-Sanchez, J.A. Reyes-Aguilera, C. Molina, **G. de la Rosa***

Hawaii Convention Center
Halls I, II, III

Functional Molecular Materials and Devices (#128)

Organized by: R. Kato, H. Mori, J. Schlueter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya

Presiding: R. Kato

Poster Session
19:00 – 21:00

- 2603.** Designing molecular printboards: A photolithographic platform for recordable surfaces. **D. Abt**, B.V. Schmidt, O. Pop-Gegeski, A. Quick, M. Wegener, D. Danilov, W. Wenzel, N.Y. Kostina, M. Bruns, C. Rodriguez-Emmenegger, C. Barner-Kowollik
- 2604.** Thermo- and photo-responsible coloring phenomena in a long-chain amidoamine derivative/toluene/water system. **K. Akazawa**, M. Nakagawa, Y. IMURA, T. Kawai
- 2605.** Influence of different modification ways on the sedimentation behavior of boron nitride applied in coating systems. **N. Andraschek***, G. Riess, W. Kern
- 2606.** Structural study on fused heterocyclic ladder oligomers. P. Pham, **M.M. Bader**
- 2607.** Molecular rectification of ferrocenyl-terminated self-assembled monolayers formed on Au(111) and Si(111). **A. Cheng***, S. Sugiura, T. Ichii, T. Utsunomiya, H. Sugimura
- 2608.** Approaching sub 100 K band-like transport in organic single-crystal transistors. **J. Cho***, H. Minemawari, H. Watanabe, T. Yamada, S. Inoue, J. Tsutsumi, S. Arai, T. Hasegawa, T. Mori
- 2609.** Electrically switchable surface with adherable, bactericidal, and nonfouling properties. **I. Choi**, W. Yeo*

- 2610.** Chiral-optical switching in a mixture system of photo-responsive rod-like molecule and achiral bent-core molecule. **S. Choi**
- 2611.** Metallic state of single-component π -molecular crystals under high pressure. **H. Cui**, R. Kato
- 2612.** From blue to red, the way to tailor exciplex based TADF emitters. **P. Data**, P. Pander, A. Monkman
- 2613.** Single-crystal linear conjugated polyenes through photoinduced inclusion polymerization: A possible organic superconductor. **S.A. Dinca**, D. Allis, M.B. Sponsler, B. Hudson
- 2614.** Air-stable ambipolar organic transistors based on layered molecular conductors (dibenzo[2,2b]pyrrolone)(dimethylidy)cyanooquinodimine). **C. Fujisue***, T. Mori, T. Kawamoto, T. Kadoya, T. Higashino
- 2615.** Preparation, characterization, and fabrication of organic thin films of porphyrin with carboxyl and phosphonate end groups. **Y. Funaki**, S. Uemura, A. Sawano, C. Pac, H. Moriyama*
- 2616.** Spin dynamics for donor-acceptor type covalent organic framework (COF). **K. Furukawa***, T. Nakamura, D. Jiang
- 2617.** Intensity adhesivity between epoxy and EC tag supported metal surface. **R. Furuno**, Y. Takatsuji, T. Haruyama
- 2618.** Synthesis and property of C5-azobenzene-functionalized locked nucleic acid uridine as a photoswitchable nucleic acid material. **O. Hasegawa**
- 2619.** Air-stable ambipolar and n-channel organic transistors with hydrogen-bond and sulfur-sulfur networks. **T. Higashino***, S. Kumeta, S. Tamura, Y. Ando, K. Ohmori, K. Suzuki, A. Filatov-Furcate, D.M. LORCY, T. Mori
- 2620.** Structural characteristics of new quantum spin liquid candidate κ -(ET)₂Ag₂[CN]₃. **T. Hiramatsu***, Y. Shimizu, M. Maesato, A. Otsuka, H. Yamochi, H. Ito, H. Kishida, Y. Yoshida, G. Saito
- 2621.** Development of piceno[4,3-b:9,10-b']diethiophene (PIDT) and alkyl substituted PIDTs (C_n -PIDTs): Synthesis, characterization, and application to organic field-effect transistors. **K. Hyodo**, R. Toyama, H. Mori, Y. Nishihara*
- 2622.** Carrier doping in a molecule-based spin ladder, L_2 [18crown-6][Ni(dmit)₂](H₂O)₄, by using solid state ion exchange. **K. Ichihashi**, S. Nishihara*, D. Konno, K. Maryunina, A. Sasaki, S. Wimperis, S. Kawaguchi, Y. Kubota, K. Inoue*, T. Akutagawa, T. Nakamura
- 2623.** Morphological control of aggregates formed from mixtures of ferrocene-containing surfactants using electrochemical methods. **A. Ikeda**, Y. Takahashi, Y. Kondo*
- 2624.** Synthesis of polynorbornene dendrimers to apply to novel thiole-one UV curable resins. **R. Imanishi**, K. Aoki
- 2625.** Discovery of thermally-resistant gold-colored crystals formed from an azobenzene derivative. **Y. Imazu**, Y. Takahashi, Y. Kondo*
- 2626.** Mott insulator κ -(ET)₂CF₃SO₃ having quasi-1D triangular spin lattice exhibiting superconducting transition under pressure. **H. Ito***, T. Asai, Y. Shimizu, Y. Yoshida, G. Saito
- 2627.** Analysis of sublimation purification process of organic semiconductor materials. **T. Iwao**, Y. Yamaguchi, Y. Tsuji*
- 2628.** New patterning process of Poly (3,4-ethylenedioxythiophene)/poly(styrenesulfonate) electrodes by using the doctor blade coating system. **Y. Jang**, K. Kim
- 2629.** Novel solvent effects of dendritic polycinnamates on the photochemical behaviors based on the dendrimer conformation in dilute solutions. **K. Kagamihara**, K. Aoki
- 2630.** Correlations between magnetism and conductivity in quasi-one-dimensional π -d molecular conductors (DIETSe),FeBr_xCl_{4(1-x)}. **G. Kawaguchi***, M. Maesato, T. Komatsu, H. Kitagawa, T. Imakubo, A. Kiswandhi, D. Graf, J. Brooks
- 2631.** Molecular coating of molds and dies for polymer processing. **B. Kaynak***, S. Waschke, G. Grundmeier, W. Kern
- 2632.** Photoresponsive carbohydrate-based amphiphilic surfactant for liquid crystal alignment. **D. Kim***, K. JEONG*
- 2633.** Dynamic and mechanical manipulation of fluidic species using a hierarchical wrinkle structure. **T. Kimura**, Y. IMURA, H. Endo, T. Kawai
- 2634.** Energy transfer through circular porphyrin arrays arranged along normally oriented cylindrical phase segregation interface in thin film. **A. Kobayashi**, Y. Tanio, T. Tokuoka, M. Aotani, S. Asaoka*
- 2635.** Preparation and redox-responsive behavior of ferrocene-modified microparticles. **N. Kobayashi**, Y. Takahashi, Y. Kondo*
- 2636.** Effect of chemical structures of amino acid-based diacetylene gelators on gelation and photopolymerization behaviors. **Y. Kobayashi**, N. Tamaoki, K. Aoki
- 2637.** Flame inhibition mechanisms of vanadocene. **Y. Koshiba***, T. Takahashi, H. Ohtani
- 2638.** Functionalized phage nanoparticles: Versatile ultrasensitive reporters for the detection of proteins and viruses. **K. Kourentzi**, M. Adhikari, S. Dhamane, J. Litvinov, H. Goux, J. Kim, H. Chen, G. Garvey, M. Crum, A. Hagstrom, U. Strych, J. Conrad, R.C. Willson*
- 2639.** Structure and physical properties of axially substituted tetramethylporphyrin radical crystals. **M. Kurokawa**, H. Hasegawa, Y. Takahashi, J. Harada, T. Inabe
- 2640.** Transport noise measurements in dimethyl-Mott insulator β' -(BEDT-TTF)₂Cl₂. **M. Kurosu**, B. Hartmann, J. Müller, J. Kudo, S. Iguchi, H. Taniguchi, T. Sasaki
- 2641.** Synthesis, structure, and emission property of polymethylene-vaulted *trans*-bis(2-iminomimidazolato)platinum(II) complexes. **N. Lee***, N. Komiya, T. Naota
- 2642.** Solution processable star-shaped molecules with a triazine core and branching thiénylenevinylenes for bulk heterojunction solar cells. **R. Lee***, C. Huang
- 2643.** Influence of electron donor groups in arylithiophene chromophores for molecular rotors. **S. Lee**, S. Lee, J. Choi, C. Lee, O. Kwon*
- 2644.** New kind of materials for Organic light-emitting diode with solution-processed. **X. Liu***, Y. Lee, S. Lee, Y. Cheon, Y. Kim
- 2645.** Organic field-effect transistors based on isoindigo derivatives. **N. Masuda***, T. Higashino, T. Kadoya, M. Ashizawa, T. Kawamoto, H. MATSUMOTO, T. Mori
- 2646.** Synthesis and photochemical behaviors of novel dendritic polycinnamates with various p-alkoxy chains in dilute solutions. **Y. Masuda**, Y. Tani, K. Aoki
- 2647.** Introduction of asymmetry in charge transfer complexes based on axially substituted iron phthalocyanine for constructing new molecular ferroelectrics. **M. Matsuda***, M. Nishi, N. Hanasaki
- 2648.** Magnetic properties of tetramethylporphyrinatocobalt(II) crystals and thin films. **S. Matsuno**, H. Hasegawa, Y. Takahashi, T. Inabe*, H. Tseng, S. Heutz
- 2649.** Current-induced mutual conductivity change along orthogonal crystal axes in an ion-radical salt of cyclophane-type donor. **M.M. Matsushita***, D. Tonouchi, K. Awaga, T. Sugawara
- 2650.** Functionalized isoindigo small molecules for use as electron acceptors in OPV devices. **S. McAfee**, J.M. Topple, I.G. Hill, G. Welch*
- 2651.** Structures and proton conductivities of novel organic anhydrous co-crystals consisting of imidazole derivatives and dicarboxylic acids. **H. Mori***, K. Suzuki, J. Yoshida, A. Ueda
- 2652.** Development of catechol-fused TTF-based organic conductors: Modulation of hydrogen-bonding interactions by chemical modification of TTF skeleton. J. Yoshida, A. Ueda, A. Nakao, R. Kumai, H. Nakao, Y. Murakami, **H. Mori**
- 2653.** Development of photo-switchable oligonucleotides containing C5-azobenzene-substituted 2'-deoxyuridine analogs. **S. Mori**, K. Morihiro*, Y. Kasahara, S. Tsunoda, S. Obika*
- 2654.** Distyrylthieno[3,2-b]thiophene based red luminescent organic single crystal and its balanced ambipolar field-effect performance. **S. Mu***, S. Takaishi, M. Yamashita
- 2655.** Synthesis and photochemical behaviors of novel photodimerizable dendrimers with stilbene and cinnamate units at their terminal positions. **S. Nakada**, Y. Tani, K. Yamauchi, K. Aoki
- 2656.** Dinaphthobenz[1,2-b:4,5-b']difurans: Synthesis, properties, and application to organic field-effect transistors. **K. Nakano***
- 2657.** Calorimetry organic charge transfer complexes under external pressures. **Y. Nakazawa***, R. Yoshimoto, S. Yamashita, H. Akutsu
- 2658.** Novel odd/even effect of alkylene chain length of diacetylene gelators on molecular packing modes in gel states to affect subsequent photopolymerization behaviors. **K. Narasaki**, N. Tamaoki, K. Aoki
- 2659.** New single crystal growth method for a charge-transfer complex using photoirradiation. **M. Nishi**, M. Matsuda, H. Hasegawa, N. Hoshino, T. Akutagawa
- 2660.** Polarization switching and domain formation of inorganic-organic lead halide perovskite thin film solar cells. **S. Oh**, G. Kim, B. Nguyen, W. Jo*
- 2661.** Crystal structure and physical properties of [Ni(dmit)₂]⁺ salt with (*p*-phenylenediamine)₂(H⁺)₃(DCH[18]crown-6)₂ double-decker type supramolecular cation. **Y. Ohshima***, K. Kubo, S. Noro, T. Akutagawa, T. Nakamura
- 2662.** Chalcogen-bridged V-shaped organic semiconductors: The effect of the bridged chalcogene atoms. **T. Okamoto***, C. Mitsui, M. Yamagishi, K. Nakahara, J. Soeda, H. SATO, A. Yamano, J. Takeya
- 2663.** Spin susceptibility of a Mott insulator k -(ET)₂Ag₂[CN]₃ with triangular lattice under pressure. **A. Ono**, Y. Shimizu, M. Itoh, M. Maesato, A. Otsuka, H. Yamochi, T. Hiramatsu, Y. Yoshida, G. Saito
- 2664.** Confinement and jamming: The result of merging the complex world of conjugated polymers, fungal Janus surfactants and colloids. **C. Rosu***, N. Kleinheinz, D. Choi, C. Tassone, J. Fu, M. Srinivasarao, P.S. Russo, E. Reichmanis
- 2665.** Photoswitching devices consisting of a metal-nanoparticle. **S. Ryuzaki***, K. Terada, N. Saito, K. Okamoto, K. TAMADA*
- 2666.** Photo-excited electron-pass from swingable molecular layer to semiconductor electrode. **T. Sakakura**, Y. Takatsuji, N. Murakami, T. Haruyama
- 2667.** Peptides: A step toward natural organic light emitting materials in electronic applications. **R. Sammyainen***, R. Bauer, G. Chang, M. Reaney, P. Jadhav
- 2668.** Organic transistors based on charge-transfer complexes of BTBT analogs. **R. Sato***, M. Dogishi, T. Higashino, T. Kadoya, T. Kawamoto, T. Mori

* Principle Author

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<http://pacifichem.org/onlineprogram>

- 2669.** Charge conduction properties at the contact interface between electron donor and acceptor single crystals.
T. Shimada*, Y. Takahashi, J. Harada, H. Hasegawa, T. Inabe
- 2670.** Antiferromagnetic order at 101 K in Mott insulator (BEDT-TTF)Ag₄(CN)₅ with diamond lattice.
Y. Shimizu*, A. Ono, M. Itoh, A. Otsuka, M. Maesato, H. Yamochi, T. Hiramatsu, Y. Yoshida, G. Saito
- 2671.** Large-scale synthesis of novel photo-reactive dendrimers with multiple azobenzene units and their photoisomerization behaviors in films.
M. Shimoyama, K. Aoki
- 2672.** Structure-property relationships in biobased polyimide copolymers derived from 4-aminocinnamic photodimer and various tetracarboxylic dianhydrides.
H. SHIN, S. TATEYAMA, T. Kaneko
- 2673.** Materials design based on the concept of coupling density.
K. Shizu, M. Uejima, H. Tanaka, T. Sato, K. Tanaka, H. Kaji, C. Adachi*
- 2674.** Light-induced superconductivity in an organic Mott insulator utilizing a photo-active electric double layer.
M. Suda*, R. Kato, H.M. Yamamoto
- 2675.** Structural stability of bismuth-niobium-oxide films in solution process.
A. Sugiyama, T. Mitani, A. Goto, H. Shimauchi
- 2676.** Development of high conductive PEDOT-PSS composite rigid film using polymerizable polar monomer.
K. Sunata, M. Horikawa, T. Shiroasaki, H. Sakurai, S. Nagaoaka, H. Ibara
- 2677.** Photopatterning of pi-conjugated polydiacetylene polymers by using organogelators with excellent photopolymerizability.
D. Takahashi, K. Narazaki, N. Tamaoki, K. Aoki
- 2678.** Synthesis and properties of novel donor-acceptor pi-conjugated dyes with high molecular planarity.
K. Takahashi, D. Izutsu, M. Wakayama, N. Tanaka, K. Mitsuke, M. Hashimoto
- 2679.** Formation of a highly ordered thin film of ferroelectric on a molecular crystal.
M. Takehisa*, Y. Takahashi, J. Harada, H. Hasegawa, T. Inabe
- 2680.** Effect of structural deformation on charge transport in organic single-crystal semiconductors.
J. Takeya*, H. Matsui, T. Kubo, R. Hausermann
- 2681.** Fabrication of color microlens array utilizing polymer electrodeposition.
T. Tanaka, K. Sato, S. Hatakeyama, M. Yamamura, S. Murakami, H. Enomoto, Y. Sakurai
- 2682.** Synthesis of novel dendritic polycinnamates with rigid tails to apply to photo-reactive films with high photodimerizable efficiency.
Y. Toyooka, Y. Tani, K. Yamouchi, K. Aoki
- 2683.** Synthesis and semiconducting properties of oxacenes containing a benz[2,1-b:3,4-b']difuran skeleton.
A.M. Truong, K. Nakano*
- 2684.** Synthesis and physical properties of 1,4,5,8-naphthalenediimide-based conductors.
K. Ueno, H. Iguchi*, M. Yamashita*
- 2685.** Effect of chemical structures of aromatic terminals of the amino-acid based diacetylene gelators on the gelation and photopolymerization behaviors.
M. Ueta, Y. Kobayashi, N. Tamaoki, K. Aoki
- 2686.** Synthesis of novel p-conjugated oligomers containing a thieno[3,4-b]thiophene unit with a 4-substituted phenyl ester and their application to solution-processed organic solar cells.
Y. Wada*, Y. Asada, T. Yamamoto, T. Ikai, K. Maeda, T. Kuwabara, K. Takahashi, S. Kanoh
- 2687.** Triethoxysilylalkyl-fluorinatedphenyl-methanimine self assembled monolayers as molecular rectifiers.
M.E. Welker*, O. Jurchescu*, Z. Lampert, A. Broadnax, L. Mendenhall

- 2688.** Temperature-mediated polymorphism in 7,14-bis(trimethylsilyl)ethynyl)dibenzo-[b,def]-chrysene: Single crystal X-ray determination of two distinct packing motifs and the impact on charge transport.
R.M. Williamson, G.E. Collis*, O. Jurchescu*, V. Coropceanu*, J. Bredas, A. Fonari, Y. Shu, K. Goetz, L. Stevens
- 2689.** Roll-to-roll fabrication of conductive polymer nanosheets and their application as skin-contact electrodes.
K. Yamagishi*, T. Fujie, A. Zucca, V. Mattoli, F. Greco, S. Takeoka

- 2690.** Switching of transfer characteristics of organic field effect transistor by phase transitions.
S. Yokokura*, Y. Takahashi, H. Hasegawa, J. Harada, T. Inabe, H. Okamoto, M.M. Matsushita, K. Awaga
- 2691.** Coronene-based cation radical salts with segregated columns.
Y. Yoshida*, K. Isomura, H. Kishida, Y. Kumagai, M. Mizuno, M. Sakata, T. Koretsune, Y. Nakano, H. Yamochi, M. Maesato, G. Saito
- 2692.** Thermodynamics study of magnetic properties in bilayer Mott insulators.
R. Yoshimoto, S. Yamashita, Y. Nakazawa, T. Kusamoto, R. Kato
- 2693.** Self-healing electronic nanodevices.
L. Zhang, X. Chen
- 2694.** Electrical transport property of nano carbon superconductors.
Y. Matsuda*, S. Heguri, K. Tanigaki

Hawaii Convention Center
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Carbon Nanotubes: Preparation, Characterization and Applications (#227)

Organized by: S. Maruyama, R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: H. Cheng, S. Maruyama

- 19:00 – 2695.** Selective growth of semiconducting single-walled carbon nanotubes.
J. Li, P. Li*, J. Liu
- 19:30 – 2696.** Development of n-type carbon nanotubes for thermoelectric materials.
T. Fujiiya, N. Nakashima, T. Fukumaru, H. Wenxin
- 19:50 – 2697.** Carbon nanotubes for energy storage.
Y. Lee

Hawaii Convention Center
318A

Advances in Bioinspired and Biomedical Materials (#245)

Organized by: K. Healy, Y. Ito, P. Messersmith, X. Chen, I. Kang
Presiding: Y. Ito

- 19:00 – 2698.** Bioinspired design of dynamic and self-healing polymers.
Z.M. Guan*
- 19:40 – 2699.** Liquid transport regularity of freeze-dried gel-like capillaries.
K. Sugaya, D. Ishii
- 20:00 – 2700.** Rationally designed dynamic protein hydrogels with reversibly tunable mechanical properties.
H. Li*, N. Kong
- 20:20 – 2701.** Novel approach for creating functional silk fibroin-based materials.
T. Hashimoto, Y. Nakamura, H. Ishikawa, T. Kameda, Y. Tamada, H. Kurosu
- 20:40 – 2702.** Injectable nanocomposite scaffold with in situ solidification and pore formation for bone tissue engineering.
P. Zhang*, N. Zhang, J. Liu, X. Chen

Hawaii Convention Center
Halls I, II, III

Challenge for Rare Element-free Functional Materials (#291)

Organized by: H. Hosono, D. Ginley, Y. Lee

Poster Session 19:00 – 21:00

- 2703.** Low-temperature synthesis of alkali niobate-based nanocomposites by solvothermal solidification method.
K. Fukasawa, S. Ueno, K. Nakashima, S. Wada*
- 2704.** Preparation and dielectric property of barium titanate ceramics by solvothermal solidification method.
H. Kawashima, S. Ueno, K. Nakashima, S. Wada
- 2705.** Preparation of insulator/lanthanum nickel oxide composite ceramics by solvothermal method and their dielectric properties.
Y. Sakamoto*, S. Ueno, K. Nakashima, S. Wada*
- 2706.** Microstructure dependence of piezoelectric properties for barium titanate ceramics prepared from different starting materials for energy harvesting application.
G.P. Khanal, E. Kobayashi, S. Ueno, K. Nakashima, S. Wada*

- 2707.** Development of new Bi-based dielectric materials with high-dielectric constant and DC-bias-free properties by nano-domain engineering.
H. Maruyama, S. Ueno, K. Nakashima, I. Fujii, S. Wada*
- 2708.** Preparation of new piezoelectric ceramics by a solvothermal solidification method under DC electric-field.
Y. Endo, S. Ueno, K. Nakashima, S. Wada*
- 2709.** Development of defect-less Bi-based piezoelectric materials with nano/macro complex domain configuration for piezoelectric enhancement.
R. Iizuka, S. Ueno, K. Nakashima, I. Fujii, Y. Kuroiwa, C. Moriyoshi, S. Wada
- 2710.** Widened process window in fabrication of Nb-doped anatase TiO₂ transparent conductive thin films by two-step annealing.
S. Nakao*, Y. Hirose, T. Hasegawa

Hawaii Convention Center
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Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei, A. Wee, W. Chen, P. Weiss
Presiding: F. Rosei

- 19:00 – 2711.** Surface-confined self-assembled Janus tectons: A versatile platform for the noncovalent functionalization of graphene.
P. DU, D. KREHER, F. MATHEVET, F. CHARRA, A. ATTIAS*
- 19:30 – 2712.** Self-assembly of heptazine derivatives at solution-electrode interfaces under electrochemical control.
S. Uemura*, Y. Nakamura, M. Kunitake
- 19:50 – 2713.** Local conformational switching of supramolecular networks at the solid/liquid interface.
F.P. Cometto*, K. Kern, M. Lingenfelder*
- 20:10 – 2714.** Surface modified with supramolecular assemblies and its electrochemical responsiveness.
J. Yuan*
- 20:30 – 2715.** Je t'aime . . . moi non plus, or how molecular self-assembly reveals the electronic properties of metal-organic interfaces.
G. Costantini*

Hawaii Convention Center
319A

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

Organized by: Z. Ye, C. Brown, T. Kiguchi
Presiding: T. Kiguchi

- 19:00 – 2716.** High piezoelectric thin films on a Si substrate from molecular-designed precursor solution.
H. Suzuki*, T. Arai, T. Ohno, N. Sakamoto, N. Wakuya
- 19:25 – 2717.** Sol-gel grown PMN-PT films for tunable bulk acoustic wave resonators.
D. Suvorov*, A. Veber, Š. Kunej, M. Spreitzer
- 19:40 – 2718.** Ferroelectric orthorhombic Me_xFe_{2-x}O₃ (Me = Al, Sc, In) thin films.
Y. Hamasaki, A. Konishi, H. Moriwake, S. Yasui, M. Itoh, T. Tanigama

- 19:55 – 2719.** Ferroelectricity in HfO₂-based epitaxial thin film.
T. Shimizu, K. Katayama, T. Shiraishi, T. Kiguchi, S. Nakamura, T.J. Konno, H. Funakubo*
- 20:20 – 2720.** Effect of gold nanoparticles on microstructure and dielectric properties of 0.93PZN-0.07BT ceramics.
A.N. Ananta, P.N. Pakawanit*, A.N. Ngmjaruojana, A.N. Rugmai
- 20:35 – 2721.** Domain structure and piezoelectric response of self-assembled tetragonal Pb(Zr,Ti)O₃ nanorods.
T. Yamada*, D. Ito, O. Sakata, T. Kiguchi, T. Shiraishi, T. Shimizu, M. Yoshino, H. Funakubo, T. Nagasaki

Hawaii Convention Center
Halls I, II, III

Self-organization: Novel Mesogens and Applications (#447)

Organized by: H. Eichhorn, E. Choi, T. Hegmann, Y. Shimizu, K. Zhao
Presiding: H. Eichhorn

Poster Session 19:00 – 21:00

- 2722.** Three-chain triphenylene discotic liquid crystals: Perfluoroalkyl induced highly ordered lamellar columnar architectures.
K. Zhao, P. Hu, B. Wang
- 2723.** Alignment control of anisotropic dye molecules induced by photopolymerization with spatially gradient light.
M. Aizawa, K. Hisano, A. Shishido*
- 2724.** Preparation of room temperature columnar liquid crystals using single hydrogen bonding of isoquinoline derivatives.
I. Son, J. Kim, J. Lee*
- 2725.** Structural chemical study on high thermal conductivity mechanism of the phenylbenzoate twin-mesogen epoxy polymer.
Y. Itoh, N. Nishimura, T. Kawai
- 2726.** Synthesis of liquid crystalline gold nanoparticles and measurement of their physical properties. I. Yuta, K. Kaneko, T. Hanasaki
- 2727.** Synthesis and investigating thermal properties of supramolecular complexes containing nucleic acid bases.
S. YOSHIKAI, K. Kaneko, T. Hanasaki
- 2728.** Comparison of photoinduced molecular reorientation in bulk and at the near-surface of photoaligned liquid crystalline polymeric films.
Y. Taniguchi, Y. Inada, M. Kondo, Y. Haruyama, S. Matsui, N. Kawatsuki*
- 2729.** Nanostructure of amphiphilic diblock copolymer thin film composed of hydrophobic side-chain liquid crystalline segment having peryleneimide mesogens.
S. Tsujimura, M. Otani, S. Asaoka*
- 2730.** Segregation of smectic phases in the binary mixture of rod-like polymers with different diameters.
K. Itsuki*, T. TANAKA, K. OKOSHI
- 2731.** Depletion effect on formation of microsegregated smectic phase.
T. TANAKA*, K. Itsuki, K. OKOSHI
- 2732.** Study on high thermal conductivity mechanism of biphenyl benzoate twin-mesogen epoxy polymer.
Y. Itoh, T. Suzuki, T. Kawai
- 2733.** Synthesis and physical properties of H-shaped liquid crystalline siloxane dimers.
A. Mori, M. Hatta, T. Shimada, K. Kaneko, T. Hanasaki

* Principle Author

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- 2734.** Mechanochromic photoluminescence behavior of liquid-crystalline rodlike oligothiophene derivatives. **T. Nakanishi***, M. Kondo, N. Kawatsuki
2735. Facile fabrication of photoalignable films fabricated from polymethacrylate with 4-oxybenzaldehyde side groups and 4-methoxyaniline composites. **K. Miyake**, M. Kondo, N. Kawatsuki*
2736. Effect of methyl substituents on the mechanochromic photoluminescent behavior of β -ciano-4-stilbazole derivatives connected with tolane moiety. **S. Miura***, M. Hashimoto, M. Kondo, N. Kawatsuki
2737. Self-organization and cross-linking of tetraazaporphyrin derivatives. **H. Eichhorn***, M. Ahmida, S. Dufour, C.E. DeWolf
2738. Comparison of photoinduced phase transitions of simple azobenzene derivatives to those of triphenylene-azobenzene derivatives. **R. Minobe**, D. Tanaka, Y. Shimizu, K. Uchida*
2739. Unusual photoswitching behavior of helical twisting power from dimeric chiral azobenzene dopants in cholesteric liquid crystal. **Y. Kim**, N. Tamaoki*
2740. Liquid crystalline properties and photochemical behaviors of amphiphilic nematic liquid crystalline diblock copolymers containing photo-crosslinkable mesogens. **S. Kubo***, S. Kobayashi, N. Kawatsuki, M. Nakagawa
2741. Synthesis and physico-chemical properties of perfluoroalkyl compounds incorporating a hexamethylene spacer. **M. Kirki**, H. OKAMOTO*, Y. MORITA
2742. Electrorheological effect of side-on liquid crystalline silsesquioxanes in a nematic solvent. **K. Kaneko**, M. Hatta, T. Shirimada, T. Hanasaki
2743. Thermal amplification of the photoinduced orientation of copoly(methacrylate) films comprised of 4-oxybenzaldehyde and benzoic acid side groups doped with 4-methoxyaniline. **R. Fujii**, M. Kondo, N. Kawatsuki*
2744. Molecular alignment by photopolymerization induced diffusion. **K. Hisano**, W. Nakano, A. Shishido*

Sunday Morning

- Hawaii Convention Center
317A
Organic, Inorganic and Hybrid Nanoparticles: Synthesis, Characterization, and Applications (#23)
Organized by: L. Bronstein, F. Winnik, K. Akiyoshi
Presiding: L. Prodi, E. Zubarev
8:00 – 2745. Fluorescent conjugated polymer nanoparticles of controlled shape, size, colour and surface functionality. **M.L. Turner***, D. Muenmart, A.B. Foster, A. Harvey, J.A. Esquivel Guzman, H. Willcock, R. O'Reilly, M. McCairn, J.M. Behrendt
8:15 – 2746. Synthesis and characterization of organically modified nanosilicon. **J.A. Irvin***, **D.J. Irvin***, L. Wood, K.L. Williams, M.A. Solano, S.K. Collings
8:30 – 2747. Photoresponsive DNA brush surface for the reversible aggregation of gold nanoparticles. **N. Kanayama***, S. Kishi, T. Takarada, M. Maeda
8:45 – 2748. Dye-doped silica nanoparticles as luminescent organized systems for nanomedicine. **L. Prodì***, E. Rampazzo, N. Zuccheroni
9:10 – 2749. Energy-gap engineering of nanosilicon toward efficient light emitters. **N. Shirahata**
9:35 – 2750. Evaporative self-assembly as a powerful tool for creating functional superstructures. **E. Zubarev***
10:00 Intermission
10:15 – 2751. Toward an understanding of halogen mediated chemistry of colloidal germanium nanocrystals. **S.M. Kauzlarich***
10:40 – 2752. Detecting, visualizing, and measuring the chirality of chiral ligand capped gold nanoparticles using nematic liquid crystal phases. **T. Hegmann***

- 10:55 – 2753.** Preparation, characterization, and application of chiral molecule-stabilized noble-metal colloids. **M. Takase***, S. Kimura, B. Ohtani
11:10 – 2754. Air-stable anisotropic monocrystalline nickel nanorods for aeronautical applications. **G.L. Drisko***, P. Fazzini, P. Fau, M. Kahn
11:25 – 2755. Synthesis, characterisation, and application of novel high attachment density nanoparticles. D. Mangos, C. Hassam, T. Nakanishi, **D.A. Lewis***
11:40 – 2756. Silicon nanoparticles: New surfaces through mechanochemistry. **M. Fink***
Hawaii Convention Center
316A
Chemistry and Applications of Graphene (#39)
Organized by: Y. Chen, R. Haddon, K. Loh
Presiding: Y. Chen, X. Gao, R. Kaner
8:00 – 2757. Nucleic acid nanotechnology for biosensing and therapy based on graphene oxide: Toward practical applications. **D. Min**
8:20 – 2758. Multiple addition reactions of π -conjugated nanocarbons. **X. Gao***
8:40 – 2759. Thick and thin film polymer-graphene nanocomposites: Surface functionalization, characterization, and applications. **Y. Park***, S. Mun, J. Park
8:55 – 2760. Flexible graphene electrode-based organic photovoltaics with record-high efficiency. **H. Park***, S. Chang, X. Zhou, J. Kong, T. Palacios, S. Gradeck
9:10 – 2761. Controllable molecular intercalation of carbon nanotubes: Toward high-yield and low-acid-use production of graphene nanoribbons. **J. Liao***, Y. Li, K. Lin, W. Chiang
9:25 Break
9:45 – 2762. Graphene-based supercapacitors for integrated energy storage. **R. Kaner***, M. El-Kady, J. Hwang, L. Wang, Y. Shao, M. Li, H. Wang, W. Sun
10:05 – 2763. Bulk 3D graphene materials. **Y. Chen**
10:25 – 2764. Applications of super-aligned carbon nanotube film in graphene research. **P. Liu***, K. Jiang
10:45 – 2765. Graphene flakes and their applications for energy storages and transparent flexible conductive films. **H. Lee***
11:05 – 2766. Roll-to-roll production and etching-free transfer of graphene for high-performance flexible transparent electrodes. **B. Deng**, z. Liu, H. Peng*
11:20 – 2767. Roll-to-roll continuous patterning and transfer of graphene via dispersive adhesion. **T. Choi***, S. Park*, J. Seo, B. Hong
Hawaii Convention Center
321A
Metal-oxo Clusters: Molecular Design from Monomers to Infinity (#79)
Organized by: M. Nyman, Y. Li, T. Ozeki, C. Ritchie
Presiding: C. Ritchie
8:00 – 2768. Polyoxometalate complexes with coordinated main group elements (Pb and Bi). **S.A. Adonin***, L. Udalova
8:20 – 2769. Chemical and electrochemical condensation of polyoxometalates with nanocrystals for solution processing electrochromic "smart windows". **D.J. Milliron***, A. Llordes, G. LeBlanc, Y. Wang
8:40 – 2770. Vanadium-based polyoxometalate as cathode-active materials for Li-ion batteries. **P.A. Aparicio***, T. Yamada, X. Lopez, H. Yoshikawa, J. Poblet, S. Irle, K. Awaga
9:00 – 2771. Oxohydroxometal clusters: Speciation, film properties, and nanopatterning. **D.A. Kesler**
9:25 – 2772. Reversible light-driven polymerization of polyoxometalate tethered with coumarin molecules. **Y. Song**
9:45 – 2773. Probing ion-pairing trends of polyoxometalates with counter-cation ^{133}Cs NMR. **D.J. Sures***, S. Sahu, A. Navrotsky, M. Nyman
10:05 – 2774. Selective uptake of Cs^+ by porous ionic crystals based on redox of polyoxometalates. **S. Seino***, R. Kawahara, S. Uchida
10:25 – 2775. High-nuclear vanadoniobate (Nb_{48}V_3) double-decker wheel. **X. Wang**
10:45 – 2776. Hafnium-oxo clusters: The atomic structure behind high-resolution patterning. **S. Goberna Ferron***, J. Son, M. Nyman, W.H. Casey
11:05 – 2777. Polyoxytungstates in photocatalysis. **J. Poblet**
11:35 – 2778. Macroion-Macroion attraction - the roles of counterions, co-ion, and water structures. **T. Liu**
Hawaii Convention Center
321B
Luminescent Nanomaterials: Properties, Mechanisms, and Applications (#101)
Organized by: F. Vetrone, S. Kohi, D. Ma, W. Huang, L. Huang, X. Peng
8:00 – 2779. Nanoheaters and nanothermometers playing together toward applications in hyperthermia. **L. Carlos***
8:40 – 2780. Nanothermometry in the second biological window based on temperature dependent near-infrared fluorescence of rare-earth doped ceramic nanophosphors. **M. Kamimura***, T. Matsumoto, S. Suyari, K. Soga
9:00 – 2781. Lanthanide-doped nanostructures for near-infrared nanothermometry. **E. Hemmer***, M. Kamimura, F. Légaré, K. Soga, F. Vetrone
9:20 – 2782. New routes for old pals: A triple RE^{3+} -doped multicolour NaGdF_4 nanoprobe for *in vitro* (980nm-NIR) and *in vivo* (793nm-NIR) imaging and sensing. **W.F. da Silva, A. Benayas**, B. del Rosal, R. Naccache, F. Sanz-Rodriguez, F. Vetrone
9:40 – 2783. Shaping lanthanide luminescence in core-shell nanoparticles. **F. Wang***
10:20 – 2784. Application of near infrared luminescent materials for biophotonics. **K. Soga**, M. Kamimura
10:40 – 2785. Dual wavelength upconversion through excitation energy trapping in core-shell nanoparticles. **N. Johnson**, S. He, A. Almutairi*
11:00 – 2786. Engineering lanthanide-doped multifunctional nanoparticles for biomedical diagnostic and therapeutic applications. **S. He**, N. Johnson, A. Almutairi
11:20 – 2787. Lanthanide-doped upconverting nanocrystals as exceptional single-molecule imaging probes and biosensors. **B.E. Cohen***, E. Chan, D. Gargas, P. Schuck
Hawaii Convention Center
320 Theatre
Functional Molecular Materials and Devices (#128)
Organized by: R. Kato, H. Mori, J. Schlüter, B. Powell, S. Lo, H. Fujii, T. Mori, J. Takeya
Presiding: H. Fujii, J. Schlüter
8:00 – 2788. Probing the Mott physics in molecular conductors via thermal expansion. **M. de Souza**
8:25 – 2789. Playing with donor and acceptor molecules. **C. Roivira***
8:50 – 2790. Charge ordering in oxo-bridged dinuclear ruthenium mixed-valence complex by magnetic resonance investigation. **T. Nakamura***, M. Yoshida, M. Kondo, S. Masaoka
9:10 – 2791. Combining intra- and intermolecular charge transfer: towards organic multiferroics. **F. Di Maio, C. Sissa, A. Painelli***
9:35 – 2792. Using crystallographically layered materials as templates for new multiferroics. **C.D. Ling***
9:55 break
Hawaii Convention Center
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Carbon Nanotubes: Preparation, Characterization and Applications (#227)
Organized by: S. Maruyama, R. Weisman, J. Liu, Y. Lee, J. Zhang
Presiding: J. Liu, S. Maruyama
8:00 – 2798. Carbon nanomaterials for biological and energy applications. **H. Dai**
8:30 – 2799. Potential biocapability of carbon nanohorns. **M. Yudasaka***
9:00 – 2800. Advanced carbon-based nanotubes/nanocages for energy conversion and storage: Synthesis, performance, and mechanism. **Z. Hu**
9:30 – 2801. Semiconducting SWCNT: Materials, inks, and printed thin film transistors. **P.R. Malenfant***, j. Ding, Z. Li, J. Lefebvre, F. Cheng, C. Homenick, J. Dunford, N. Du, J. Ouyang, G. Lopinski, R. James, C.T. Kingston, B. Simard, J. Humes, J. Kroeger, W. Lee, J. Sun, G. Cho
9:50 break
10:10 – 2802. Dry-processable carbon nanotubes for functional devices and composites. **J. Di, Y. .Zhu, Q. Li**
10:40 – 2803. Toughness of carbon nanotube and graphene hybrid fibers. **S. Kim**
11:10 – 2804. Carbon nanotube-silver hybrid architecture for stretchable composites and fibers. **S. Baik***
11:40 – 2805. Industrialization of boron nitride nanotubes: Synthesis, chemistry, assemblies, and composites. **B. Simard**, K. Kim, C. Kingston, M.J. Jakubinek, C. Homenick, Y. Martinez-Rubi, H. Shin, B. Ashrafi, J. Guan, S. Lin, S. Denomme, R. Iannitti, S. Walker, M. Daroszewska, M. Plunkett
Hawaii Convention Center
318A
Advances in Bioinspired and Biomedical Materials (#245)
Organized by: K. Healy, Y. Ito, P. Messersmith, X. Chen, I. Kang
Presiding: X. Chen
8:00 – 2806. Design of bioactive materials for tissue regeneration. **J. Chang***
* Principle Author
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8:40 – 2807. In vitro design of nanoparticles using an artificial 3D-blood vessel wall models for atherosclerosis treatment.

M. Matsusaki*, P. Chetprayoon, M. Akashi

9:00 – 2808. Surface modification of nHA nanorods hydroxyapatite for use in tissue engineering scaffolds. A. haider*, I. Kang

9:20 – 2809. Amino acid-based poly(ester amide)s: Tunable materials for tissue engineering and drug delivery. E.R. Gillies*, K. Mequanint, D.K. Knight, A. Soleimani

9:40 Coffee Break

10:00 – 2810. Tailoring minimalist self-assembling peptides for localised viral vector gene therapy. A. Rodriguez, K. Bruggeman, C.L. Parish, R.J. Williams, D.R. Nisbet*

10:20 – 2811. Cryptic site surfaces for the design of chemo and cyto mechano-responsive systems. P. SCHAAF

11:00 – 2812. Synthetic cell penetrating peptides for drug delivery and stem cell applications. W.H. Suh*

11:20 – 2813. Strategies for the incorporation of cellobiose dehydrogenase into chitosan formulations: Antimicrobial systems for medical applications. G. Tegli*, B. Thallinger, B. Beer, G.S. Nyanhongo, G.M. Guebitz

11:40 – 2814. Bioinspired synthesis of multifunctional metal nanoparticles for biomedical applications. Y. Tan*, J. Lim, Y. Yu, X. Su

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317B

Challenge for Rare Element-free Functional Materials (#291)

Organized by: H. Hosono, D. Ginley, Y. Lee
Presiding: Y. Lee

8:00 – 2815. Low temperature preparation of barium titanate-based nano-complex ceramics by solvothermal solidification method and their dielectric and piezoelectric enhancement. S. Wada

8:20 – 2816. Low-temperature preparation of high-capacitance metal/insulator composite capacitors with boundary layer structure. S. Ueno*, Y. Sakamoto, K. Nakashima, S. Wada

8:40 – 2817. Piezoelectric Langasite single crystals for high temperature sensors. K. Shimamura*, X. Fu, E. Villora, Y. Oshima, Y. Noguchi, M. Miyayama, N. Ohashi

9:00 – 2818. Fabrication and optical characterization of plasmonic array of titanium nitride nanoparticles. R. Kamakura*, Y. Daido, S. Murai*, K. Fujita, K. Tanaka

9:20 Break

9:30 – 2819. 2D carbides of transition metals: A new class of functional materials. Y. Gogotsi*

10:00 – 2820. Synthesis of potassium niobate nanocubes using microwave-assisted solvothermal method.

K. Nakashima*, S. Ueno, S. Wada

10:20 – 2821. Progress on the applications of super-aligned carbon nanotube films.

Y. Wei, P. Liu, S. Fan, K. Jiang

10:50 – 2822. Stabilities and electronic structures of bilayer graphene doped with B and N atoms: A first-principles study.

Y. Fujimoto*, S. Saito

11:10 – 2823. Electronic and optical properties of newly discovered crystal structures of $g\text{-C}_3\text{N}_4$ by ab initio evolutionary structure search. J. Wang*, N. Umezawa

11:30 – 2824. Graphene vs. carbon nanotubes: Fundamentals and applications electronics. Y. Lee

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318B

Nitroxide Radicals: Synthesis and Functional Bio-/Nanomaterials (#309)

Organized by: A. Smirnov, S. Bottle, R. Tamura
Presiding: T. Smirnova, D.D. Thomas

8:00 – 2825. Nitroxide-loaded lipid nanoparticles provide MRI contrast in vivo.

B.W. Muir*

8:40 – 2826. Nitroxide-radical containing polymers for novel nanotherapeutics.

T. Yoshitomi, Y. Nagasaki*

9:00 – 2827. Multifunctional in vivo EPR profiling of the chemical tumor microenvironment using advanced nitroxide and trityl probes. V.V. Khramtsov*

9:30 Break

9:45 – 2828. Mechanism of (acid-catalyzed) radical-trapping antioxidant activity of nitroxides. E.A. Haidasz, D. Meng, R. Amorati, K. Ingold, L. Valgimigli*, D. Pratt*

10:15 – 2829. Multifunctional assessment of tissue pO_2 , pH and inorganic phosphate (Pi) by phosphonated trityl probe: Interstitial Pi as a new prognostic factor in tumorigenesis. A. Bobko, T.D. Eubank, I. Dhimitrula, J.L. Zweier, V.V. Khramtsov

10:45 – 2830. Grafting nitroxide radicals on nanodiamond surface using click chemistry. S. Takahashi*

11:15 – 2831. Spin labeled tachykinin neuropeptides for in-vivo imaging and determination of copper binding. I.J. berliner*, c. jones

11:45 Concluding Remarks

Supramolecular Assemblies at Surfaces: Nanopatterning, Functionality, Reactivity (#346)

Organized by: D. Perepichka, F. Rosei, A. Wee, W. Chen, P. Weiss

Presiding: S. De Feyter, F. Rosei

8:00 – 2832. Supramolecular gateways to single molecule electronic properties.

E. Bourget*

8:30 – 2833. Supramolecular assemblies on surfaces from cyano-functionalized molecules.

M. Stoehr*

9:00 – 2834. Stoichiometry and electronic structure of bidimensional donor/acceptor superlattices on metal surfaces.

R. Otero*

9:30 – 2835. Doping of graphene through physisorbed self-assembled monolayers.

R. Phillipson, J. Teysander, L. Verstraete, I. Asselberghs, S. De Gendt, J. Adisoefoso*, S. De Feyter

9:50 – 2836. N-heterocyclic carbenes on gold: Forming an ultrastable self-assembled monolayer N-heterocyclic carbenes on gold with applications in surface plasmon resonance sensors.

H. Horton*, C. Cradden, Z. Li

10:10 Coffee break

10:20 – 2837. Graphene nanoribbons produced by 2-zoned chemical vapor deposition.

H. Sakaguchi*

10:50 – 2838. Template-assisted self-assembly of MoS_x molecular wires and nanoribbons.

K.P. Loh*

11:20 – 2839. Processes at the solution-solid interface: Desorption rates and activation energy for metal free octaethylporphyrin at the phenylcokane/graphite interface.

A. Bhattacharjee, K. Hippis, U. Mazur

11:40 – 2840. Anion sensing supramolecular monolayers.

J. Lehr, T. Lang, O. Blackburn, T. Barendt, S. Faulkner, P. Beer, J. Davis*

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316C

Fundamentals and Applications of Nanomaterials for Energy Technologies (#348)

Organized by: S. Jin, G. Yu, T. Minegishi, S. Maldonado, J. He

Presiding: F. Wang, G. Yu

8:00 – 2841. 3D nanostructure electrodes for Li and Na ion batteries.

Y.I. Chen*

8:30 – 2842. Nanostructured ternary metal fluorides as new cathodes for rechargeable lithium batteries with high energy density and cycling efficiency.

F. Wang*, S. Kim, J. Graetz

8:50 – 2843. Preparation of metallic monolith using polymer template and its application to battery electrodes.

K. Mitamura*, M. Watanabe, S. Watake, K. Matsukawa

9:05 Break

9:15 – 2844. New vistas in electrochemical energy storage enabled by nanomaterials.

L. Nazar*, D. Kundu, X. Liang, R. Black, Q. Pang

9:45 – 2845. Nanostructured materials for energy storage.

J. Liu

10:15 – 2846. High-energy lithium-sulfur batteries: From theoretical understanding to nanomaterials design.

Z. Seh, W. Li, Y. Cui*

10:30 – 2847. Binder free graphene–sodium niobate nanotube/nanorod composite electrodes for supercapacitors.

W. Perera, i. munawera, M. Trinh, Y. Gao, J.p. Ferraris, Y. Chabal, K. Balkus*

10:45 – 2848. Facile synthesis of strongly coupled carbon nanofiber-metal oxide coaxial nanocables as high performance anode materials for lithium-ion batteries.

G. Zhang

11:00 – 2849. Preparation of ultrafine polyacrylonitrile-based carbon nanofibers embedded with polyvinylpyrrolidone functionalized graphene by electrospinning.

A. Moayeri*, A. Ajii

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316B

Multi-scale & Synergistic Supramolecular Systems in Material and Biomedical Sciences (#357)

Organized by: S. Aoki, H. Chiu, K. Soga, N. Gianneschi, X. Bengang

Presiding: S. Aoki, N. Gianneschi

8:00 – 2850. Systematic study of the structure–function relationship in Archaea-inspired bolaform lipids.

G. Leriche, Y. Kim, T. Koyanagi, T. Schroeder, K. Diraviam, K. Gao, M. Gilson, D. Sept, M. Mayer, J. Yang*

8:25 – 2851. Anomalous water molecules and mechanistic effects of water nanotube clusters confined to molecular porous crystals.

M. Tadokoro*

8:50 – 2852. Modulating biomaterial-surface interactions using light.

R. Naik*

9:10 – 2853. Synthesis of functionalized [2]rotaxanes from macrocyclic phenanthroline-Cu complexes.

S. Saito*, K. Ikeiyatsu, Y. Matsuoka, Y. Mutoh

9:30 Break

9:35 – 2854. Design and synthesis of heteroleptic cyclometalated iridium(III) complexes that exhibit unusual dual color phosphorescence.

S. Kumar, Y. Hisamatsu, S. Aoki*

9:55 – 2855. Rolling DNA-based motors with superdiffusive transport.

K. salaita*

10:15 – 2856. Self-assembled and stimuli responsive protein-binders.

J. Jayawickramarajah*, X. Su, X. Chu, M. Zhu

10:40 Closing Remarks

Hawaii Convention Center
319A

Synthesis, Structure and Functionalities of Ferroelectrics and Multiferroics (#432)

Organized by: Z. Ye, C. Brown,

T. Kiguchi

Presiding: J. Li

8:00 – 2857. Structure and dynamic behaviors of ferroelectric domains.

x. pan

8:25 – 2858. Atomic-resolution analysis of structure and morphology of PMN-PT epitaxial thin films.

T. Kiguchi*, C. Fan, T. Shiraishi, T.J. Konno

8:00 – 2859. Investigation of various domain wall alignments in epitaxial PbTiO₃ thin films on conducting LaNiO₃ grown by pulsed laser deposition.

H. Jin, S. Oh, W. Jo*

9:05 – 2860. Electron microscopic study on dynamics of nanoscale ferroelectric domains in Pb(Mg_{1/3}Nb_{2/3})O₃ – PbTiO₃.

Y. Sato

9:20 – 2861. Electronic transport in ferroelectric nanostructures.

A. Gruberman*

9:45 Break

9:55 – 2862. Order, disorder, and ferroic properties.

P. Janolin*, R. Faye, C. Cochard, H. Liu, O. Guedes, B. Dkhil, S. Prosandeev, L. Bellache

10:20 – 2863. Broadband dielectric spectroscopy of A-site substituted relaxor ceramics.

J. Banys*, S. Svirskas, M. Dunce, E. Birks, M. Antonova, A. Sternberg

10:35 – 2864. Phase transition driven by pulsed electric field in epitaxial piezoelectric thin films.

S. Yasui*, Y. Ehara, T. Shiraishi, T. Shimizu, H. Funakubo, M. Itoh, Y. Imai, H. Tajiri, O. Sakata, I. Takeuchi

10:50 – 2865. Aurivillius phase Bi₄Ti₃O₁₂-nBiFeO₃ (n = 1-5) single crystals compared with ceramics.

H. Kimura*, T. Jia, R. Tanahashi, H. Zhao

11:05 – 2866. Coupled ferroelectric and magnetic orders in PbFe₁2Nb₁/2O₃.

C. Stock, H. Luo, B. Roessli

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322AB

Self-organization: Novel Mesogens and Applications (#447)

Organized by: H. Eichhorn, E. Choi, T. Hegmann, Y. Shimizu, K. Zhao

Presiding: E. Choi

8:00 – 2867. Thermally reversible distortion of ABA triblock copolymer having main-chain liquid crystalline polyester as a central block.

M. Koga, K. Abe, Y. TOMINAGA, M. Tokita*

8:20 – 2868. Photodeformation of liquid crystal polymers triggered by upconversion luminescence.

Y. Yu*, Z. Jiang, W. Wu, L. Qin

8:50 – 2869. Improving and extending the dynamic optical response of polymer stabilized cholesteric liquid crystals with materials chemistry.

T.J. White*, K. Lee, V.P. Tondiglia, T.J. Bunning

9:10 – 2870. Rational molecular design for bicontinuous cubic mesogens 1,2-bis(4-n-alkoxyxloy)hydrazines.

S. Kutsumizu*, Y. Yamada, I. Tokiwa, A. Kawafuchi, T. Sugimoto, T. Udagawa, Y. Miwa

9:30 – 2871. Synthesis and mesomorphism of dimesogenic molecules with hocky stick-shaped mesogens.

E. Choi*, H. Kim

9:50 Break

9:55 – 2872. Achiral straight-rod liquid crystals indicating local biaxiality and ferroelectric switching behavior in the smectic A and nematic phases.

K. Kishikawa*, T. Inoue, N. Hasegawa, M. Takahashi, M. Kohri, T. Taniguchi, S. Kohmoto

10:15 – 2873. Emergence of chirality in chemically nonchiral nematic dimers.

G.H. Mehl*

* Principle Author

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- 10:45 – 2874.** Design of "de Vries-like" liquid crystals for fast electro-optical applications. **R. Lemieux***
- 11:15 – 2875.** Effect of dipolar interactions on chiral liquid-crystal systems. **T. Nozawa***, P. Brumby, K. Yasuoka
- 11:35 – 2876.** Design of new chiral smectic C' lyotropic liquid crystals. **C. Schubert**, R.P. Lemieux, F. Giesslmann
- 11:55 Closing Remarks**

ENRG

Area 9 – Chemistry of Clean Energy Conversion, Storage, and Production

Tuesday Morning

Hyatt Regency Waikiki
Makai Ballrm

Chemistry of Automotive Emission Control Catalysis: Current R&D and Future Challenges (#21)

Organized by: C. Peden, D. Kim,
M. Shen, W. Epling
Presiding: B. Epling, C. Peden

- 8:00 – 1.** Approaches and advances to the challenges of treating lean emissions at low temperatures. **T.J. Toops***, J.E. Parks, E. Kyriakidou, A.J. Binder
- 8:40 – 2.** CO removal from automotive emission over thermal durable CeO₂-supported Cr-Cu catalyst. **H. Yoshida**, Y. Okabe, N. Yamashita, S. Hinokuma, M. Machida*

- 9:00 – 3.** Three-way catalytic performance of Ru/Co/Al₂O₃ enhanced by preparation using a galvanic method. **J. Ohyama***, H. Ishikawa, Y. Mahara, A. Satsuma
- 9:20 – 4.** Surface structure dependence of SO₂ interaction with CeO₂ nanoshapes with well-defined facets. U. Tumuluri, M. Li, S. Dai, **Z. Wu**

- 9:40 – 5.** Catalytic combustion reaction on Mn-defined hexagonal YbFeO₃. **R. Tada***, S. Hosokawa, K. Teramura, T. Tanaka
- 10:00 – 6.** Pulsed arc-plasma deposition of noble metal nanoparticles for automotive catalytic reactions. **S. Misumi**, S. Hinokuma, H. Yoshida, M. Machida*

- 10:20 – 7.** Recycling valuable metals from automobiles: Separation of precious metals in simple extraction steps using ionic liquids. **N. Papaiconomou***, E. Chainet, I. Billard, L. Svecova
- 10:40 – 8.** Multilayer and zoned monolithic catalysts for lean NOx reduction. **M. Harold***

Hyatt Regency Waikiki
Kou Ballrm

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli
Presiding: N. Abatzoglou, A. Dalai

- 8:00** Opening Remark-Nano Catalysis for Clean Energy-I
- 8:02 – 9.** Nanoscale nickel phosphide catalysts for hydrodenitrogenation and hydrodesulfurization: In situ preparation at low temperature. **M.E. Bussell**, S. Danforth, A. d'Aquino, B.J. Morgan, T. Clinkingbeard

- 8:22 – 10.** Iron-functionalized carbon nano-filaments for hydrogen sulfide removal applications. **C. Fauteux-Lefebvre***, N. Abatzoglou
- 8:42 – 11.** Design of silica-based metal complex catalysts for activation of CH₄ and CO₂. **A. Karkamkar***

- 9:02 – 12.** Novel NiMo supported catalysts over an enwrapped composite of ZSM-5/KIT-6 for deep hydrodesulfurization. **A. Duan***, H. Wu, S. Song, d. Qi, Z. Zhao
- 9:22 – 13.** Effects of EDTA on the activity of NiMo catalysts supported on different mesoporous metal oxides for hydrotreating of heavy gas oil. **S. Badoga**, A. Dalai, J. Adjaye
- 9:42 – 14.** Class of high performance non-platinum oxygen reduction electrocatalysts based on cheap carbon blacks. **W. Xu**

- 10:02 Break**
- 10:17** Opening Remark-Nano Catalysis for Clean Energy-II
- 10:20 – 15.** New insights for catalytic deoxygenation mechanisms induced by cobalt and nickel. **Y. Zheng**, H. Zhang, **H. Lin**
- 10:40 – 16.** Confined nanocatalysis in carbon nanotubes. **X. Pan***, F. Zhang, T. Cui, X. Li, J. Yang, X. Bao*
- 11:00 – 17.** Catalytic SO₃ decomposition over supported vanadates for solar thermochemical water splitting. **T. Kawada**, A. Ikematsu, M. Sueyoshi, S. Muraoka, S. Hinokuma, M. Machida
- 11:20 – 18.** Valorization of a mining residue as a nanometric spinel catalyst for hydrocarbons reforming. **N. Abatzoglou***, M. Chamouni, F. Larachi, M. Iliuta
- 11:40 – 19.** Modification of metal catalysts with organic and inorganic thin films for energy applications. **J. Medlin**

Hyatt Regency Waikiki
Ekahi

Progress Toward a Lignocellulosic Biorefinery (#144)

Organized by: A. Stipanovic, A. Varma, Y. Sung
Presiding: A. Stipanovic

- 8:00** Arthur Stipanovic
- 8:05 – 20.** Advances in low recalcitrance plants and tailored pretreatments. **A. Ragauskas**
- 8:45 – 21.** Inducible extreme expression of cellulases in poplar. C. Poovaiah, Y. Xiao, L. Northern, **H. Coleman***
- 9:10 – 22.** Exploring glycosidase inhibitors as a tool to screen and assay glycan-degrading enzymes. **M. Zierke**, T. Rasmussen, K. Li, S.G. Withers*
- 9:30 – 23.** Supramolecular interactions and nanoscale forces in plant cell walls: Insights from the molecular theory of solvation. **S. Stoyanov**, A. Kovalenko
- 9:50 – 24.** Ambidexterous heteropolysaccharides affect on preparation of cellulose nanofibrils from different plant sources. **S. Fu***, Q. Meng, L.A. Lucia
- 10:10 – 25.** Elucidation of cell wall deconstruction by environmentally benign pretreatments using solution- and solid-state NMR spectroscopy. **K. Cheng***, A. Stipanovic*

- 10:30 – 26.** Improving the quality of lignin produced in fractionation of hardwoods based on HWE. M.J. Goundalkar*, C. Gong, P.S. Dongre, D.B. Corbett, C. Wood, C. Jing, O. Theriasme, A. Nagardeolekar, T.E. Amidon, **B.M. Bujanovic**

- 10:50 – 27.** Making sense out of chaos - catalyst design for the conversion of biorefinery lignin to high value chemicals. **J.J. Bozell***, C. Njorob, B. Biannic, T. Elder

- 11:10 – 28.** Solvent-induced decrystallization and dissolution of cellulose for efficient biomass utilization. M. Ghasemi, M. Tsianou, **P. Alexandridis***

- 11:30 – 29.** Hydrothermal pretreatment of palm oil empty fruit bunch with palm oil mill effluent: The effect of temperature. **N. Syaftika**, Y. Matsumura*

Hyatt Regency Waikiki
Elima

Dynamical Processes of Light Harvesting Surfaces (#178)

Organized by: G. Thornton, M. Henderson, H. Onishi, C. Li, G. Herman

Presiding: M.A. Henderson, G. Thornton

- 8:00** Opening Remarks
- 8:05 – 30.** Ultrafast electron photoexcitation and relaxation pathways in TiO₂ photocatalysis. **H. Petek***, A. Argondizzo

- 8:45 – 31.** Elemental processes in photocatalysis of methanol and water on TiO₂(110). **X. Yang***

- 9:15 – 32.** Hydroxyl induced unoccupied state on rutile TiO₂(110). **Y. Zhang**, D.T. Payne, C.L. Pang, H.H. Fielding, G. Thornton*

- 9:45 – 33.** Photocatalysis on TiO₂: Insights from first principles simulations. **A. Selloni**

- 10:15 – 34.** Energy and dipole dependence of heterogeneous electron transfer dynamics. **L. Gundlach***, J. Nieto-Pescador, B. Abraham

- 10:45 – 35.** X-ray studies of catalysis in artificial photosynthesis. **A. Nilsson**

- 11:15 – 36.** Photocatalysis for hydrogen production over metal supported TiO₂. A. Khan, A. Schneider, K. Wahab, S. Bashir, S. Chaeib, J.A. van Bokhoven, **H. Idriss***

Hyatt Regency Waikiki
Maloko Ballrm

Water-phase Catalysis for Energy and Chemicals Production (#182)

Organized by: M. Wong, C. Zhang, S. Jeong
Presiding: L.C. Grabow, M.S. Wong

- 8:00** Opening Remarks (5 min)

- 8:05 – 37.** Vapor-phase cyclohexene epoxidation by H₂O₂ over mesoporous TS-1. S. Kwon, N. Schweitzer, R.Q. Snurr, **P.C. Stair**

- 8:23 – 38.** Role of defect sites in the hydrolysis of cellulose and oligosaccharides over activated carbon catalysts. **C. Sievers**, G. Foo

- 8:48 – 39.** Hydrolysis of woody biomass by enzyme-mimicking carbon catalyst. **A. Fukukawa***, H. Kobayashi

- 9:06 – 40.** Impact of water on the dehydration of alcohols. **J. Lercher**

- 9:31 Break (15-min)**

- 9:46 – 41.** Lewis acid containing molecular sieve catalysts for converting sugars in aqueous media. **M.E. Davis**

- 10:11 – 42.** Stability and application of zeolite catalysts in condensed aqueous phase. **T. Ennart**, P. Jacobs, B. Sels*

- 10:29 – 43.** Catalytic conversion and production of glycerol in aqueous and organic media. **Y. Suh***

- 10:54 – 44.** Magnetic resonance spectroscopy and diffusion experiments point to multiple roles for water in reactions catalyzed by zeolites. **J.L. White**, K. Chen, J. Kelsey, D. Resasco, L. Zhang

- 11:12 – 45.** Kinetic inhibition by water of liquid-phase sugar isomerization reactions catalyzed by hydrophobic and hydrophilic Lewis acid zeolites. J.S. Bates, M.J. Cordon, J.W. Harris, J. Vega-Vila, W. Delgass, F. Ribeiro, **R. Gounder***

Hyatt Regency Waikiki
Mauka Ballrm

Artificial Photosynthesis: Reduction of Carbon Dioxide (#271)

Organized by: O. Ishitani, E. Fujita, S. Kang
Presiding: E. Fujita, S. Kang

- 8:00** Opening Remarks

- 8:05 – 46.** Selective, efficient molecular catalysis for the CO₂/CO conversion in aprotic solvent and in pure water using reduced iron porphyrins. **M. Robert***

- 8:30 – 47.** Bioinspired dinuclear iron catalysts for efficient and selective CO₂ reduction. **Y. Naruta***

- 8:55 – 48.** New platforms and polyoxometalates as electron acceptors/donors for the photoreduction of carbon dioxide. **R. Neumann**

- 9:20 – 49.** Photocatalytic CO₂ reduction systems using CO₂ capturing ability of Re(I) complexes. **T. Morimoto***

- 9:45 Break**

- 9:55 – 50.** Molecular mechanism of the photochemical CO₂ reduction sensitized by rhodium bipyridine complexes. **H. Inoue***

- 10:20 – 51.** Experimental and theoretical investigation of hydride intermediates in photocatalytic CO₂ reduction by mono-nuclear [M^{II}(tpy)(ppv)Cl]⁺ complexes. **M.Z. Ertan**, K. Garg, Y. Matsubara, S. Sato, J.T. Muckerman, E. Fujita

- 10:35 – 52.** Rapid reduction of carbon dioxide to carbon monoxide by manganese(II) diamine electocatalysts in the presence of Brønsted acids. B. Dhakal, B.A. Corbin, D.A. Kurtz, R.J. Hulme, **G.A. Felton**

- 10:50 – 53.** Mechanistic role of redox non-innocent ligands in CO₂ reduction catalysis by (bpy)M(CO)_x and (tpy)M(CO)_x system. **M. Baik**

- 11:15 – 54.** Carbon dioxide reduction by manganese bipyridine complexes: Lowering overpotentials and enhancing stability. M. Sampson, **C.P. Kubik***

- 11:40 – 55.** Design of a catalytic active site for electrochemical reduction of CO₂ to CO using am(m-)tricarbonyl based homogeneous electrocatalyst. **A.B. Bocarsly***, T.W. Shaw, J. Agarwal

Tuesday Afternoon

Hyatt Regency Waikiki
Makai Ballrm

Chemistry of Automotive Emission Control Catalysis: Current R&D and Future Challenges (#21)

Organized by: C. Peden, D. Kim, M. Shen, W. Epling
Presiding: D. Kim, M. Shen

- 13:00 – 56.** H₂-SCR of NOx over novel Pd-Au/TiO₂ catalyst. **Z. Liu***, K. Duan, L. Ma

- 13:20 – 57.** Molecular elucidation of NOx selective catalytic reduction in Cu-SSZ-13. C. Paolucci, A. Parekh, J. Miller, W. Delgass, R. Gounder, F. Ribeiro, **W.F. Schneider***

- 14:00 – 58.** Possible reaction pathway for the selective catalytic reduction of NO with NH₃ on Cu/SSZ-13 zeolite at low temperatures. **W. Su***, J. Li

- 14:20 – 59.** Recent advances in fundamental understanding of automotive NH₃-SCR reactions. **E. TRONCONI***

- 15:00 – 60.** Al rich BEA⁺ zeolites as deNO_x catalysts. **J. Dedecek**, P. Szazma, B. Wichterlova, G. Sadovska, A. Vondrova, V. Pashkova

- 15:20 – 61.** Approaching rational design of Cu- and Fe/CHA SCR catalysts. **F. Gao***, M. Kollar, Y. Wang, J. Szanyi, C. Peden

- 16:00 – 62.** Precious metal doped barium cerates as NO_x catalysts. **K. Stamm Masias***, T.C. Peck

* Principle Author

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16:20 – 63. Rh supported on metal phosphates as an efficient automotive catalyst for NO_x reduction under slightly lean conditions. H.P. Buwono, S. Minami, S. Hinokuma, H. Yoshida, Y. Nagao, Y. Nakahara, T. Sato, H. Iwakura, **M. Machida***

16:40 – 64. Oxygen storage capacity of Sr₃FeO_{7-d}. **K. Beppu***, S. Hosokawa, K. Teramura, T. Tanaka

Hyatt Regency Waikiki
Kou Ballrm

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli
Presiding: N.C. Pradhan, G.D. Yadav

13:00 Opening Remark-Environmentally Friendly Chemical Production-I

13:02 – 65. Production of hydrogen by dry reforming of ethanol over alumina-supported nano-NiO/SiO₂ catalyst. B. Bej, **N.C. Pradhan***

13:22 – 66. Mechanochemical processing for Hydrogen production from sewage sludge. **S. Ishihara***, J. Kano

13:42 – 67. Consumption of CO₂ for value-added chemicals. **S. Park***

14:02 – 68. Synthesis of AgPd core Pd shell nanocatalysts loaded on TiO₂ by microwave heating in aqueous solution for efficient hydrogen production from formic acid. **M. Tsuji***, M. Hattori, D. Shimamoto, H. Ago

14:22 – 69. High-surface-area mixed metal oxide nanocatalysts for H₂ generation. **F. Kleitz***, H. Yen

14:42 – 70. Supported gold phosphine clusters for the selective oxidation of styrene. **D.P. Anderson**, V. Golovko, G.F. Metha, G. Andersson

15:02 Break

15:17 Opening Remark-Environmentally Friendly Chemical Production-II

15:20 – 71. Isopropyl esters in a fluidized catalytic bed. **D. Boffito***, F. Galli, C. Pirola, C.L. Bianchi, G.S. Patience

15:40 – 72. Auto-reduced Cu/CNTs catalysts designed for hydrogenation of dimethyl oxalate to synthesize ethylene glycol. **P. Ai**, G. Liu, M. Tan, G. Yang, Y. Yoneymaya, N. Tsukubi*

16:00 – 73. Ruthenium catalyzed ammonia decomposition using alkaline-earth titanates as support materials. **T. Yago**, Y. Horiechi, M. Matsuoaka*

16:20 – 74. Cascade engineered synthesis of γ -valerolactone, 1,4-pentanediol and 2-methyltetrahydrofuran from levulinic acid by heterogeneous catalysis in water. **G.D. Yadav***, S. Patankar

16:40 – 75. Nanoparticle catalytic site tuning for CO₂ reduction. **w. zhu**, y. zhang, h. zhang, A. Peterson, S. Sun

Hyatt Regency Waikiki
Ekahi

Progress Toward a Lignocellulosic Biorefinery (#144)

Organized by: A. Stipanovic, A. Varma, Y. Sung
Presiding: A.J. Varma

13:00 – 76. Wet explosion pretreatment as a major step into the future of biorefineries. **B.K. Ahring***

13:20 – 77. Sustainable carbonaceous materials and chemicals via biomass hydrothermal processing. **M. Titirici***, F. Pileidis

13:40 – 78. Electron Beam pretreatment of woody biomass for enhancing the production of biofuels. **A. Stipanovic***, K. Cheng, N. Bergey, M. Driscoll

14:00 – 79. Utilization of cellulose, hemicellulose, and lignin in woody biomass. **A. Yamaguchi***, O. Sato, N. Mimura, M. Shirai

14:20 – 80. Sterically protected and electronically activated azamacrocyclic catalysts for lignin depolymerization: A new approach to biomass valorization. **M.S. Chorghade***

14:40 – 81. Catalytic and high frequency ultrasound-assisted conversions of edible and non-edible biomass to fuels. **Y.G. Adewyui***

15:00 – 82. Low-cost ionic liquids for lignocellulose deconstruction. **J.P. Hallett**, A. Brandt

15:20 – 83. Decomposition and reaction behavior of cellulose in ionic liquid. **H. Miyafuji***

15:40 – 84. Homogeneous processing of biomass with ionic liquids: Pre-treatments to avoid decomposition and preserve molecular weight. S. Deb, S. Labafzadeh, A.P. Parviainen, M. Borrega, I. Kilpeläinen, **A.W. King***

16:00 – 85. Process improvements in the fermentation of biomass-derived sugars to ethanol biofuel using electron beam technology. **N. Bergey**, A. Stipanovic

Hyatt Regency Waikiki
Elima

Dynamical Processes of Light Harvesting Surfaces (#178)

Organized by: G. Thornton, M. Henderson, H. Onishi, C. Li, G. Herman
Presiding: G. Herman, H. Onishi

13:00 – 86. Photoinduced excitation and decay of polarons studied on a ms-time-scale using IR-spectroscopy: The cases of TiO₂ and ZnO. **C. Woell***

13:30 – 87. Novel method for determination of TiO₂ midgap states: Transient infrared absorption-excitation energy scanning spectrum and its application. **Y. Weng***

14:00 – 88. Photo-generated electrons and holes transfer across the anatase/rutile TiO₂ phase junction. **X. Wang**, S. Shen, A. Kafizas, J. Durrant, C. Li*, Z. Feng

14:15 – 89. Probing charge carrier dynamics in benzoporphyrin thin films by time-resolved THz spectroscopy. **K. Ohta***, S. Hiraoaka, Y. Tamura, H. Yamada, K. Tominga

14:30 – 90. Temperature dependence in the photodesorption of small molecules from the rutile TiO₂(110) surface. **M.A. Henderson***, G. Kimmel, N. Petrik

15:00 – 91. Hot electron-driven chemical and solar energy conversion on metal-oxide nanostructures. **J.Y. Park**

15:15 – 92. New insights into photochemistry of acetone on rutile TiO₂(110). **N. Petrik***, M.A. Henderson, G. Kimmel

15:30 Break

15:40 – 93. Linker rectifiers for covalent attachment of catalysts to semiconductor surfaces. W. Ding, M. Koepf, C. Konigsmann, A. Batra, L. Venkataraman, C. Negre, G. Brudvig, R. Crabtree, C. Schmuttenmaer, **V. Batista***

16:10 – 94. Electron injection dynamics of Ru-based dye/TiO₂ system in the presence of different organic solvents: Role of solvent dipole moment and donor number. **A. Furube**, S. Mahanta, H. Matsuzaki, T.N. Murakami, R. Katoh, H. Matsumoto

16:40 – 95. Effect of interfacial energy alignment on the mechanism of electron injection in highly efficient dye-sensitized solar cells. **L. Han***, X. Yang, S. Zhang, A. Islam

Hyatt Regency Waikiki
Maloko Blrm

Water-phase Catalysis for Energy and Chemicals Production (#182)

Organized by: M. Wong, C. Zhang, S. Jeong
Presiding: A. Fukuoka, Z. Zhang

13:00 – 96. Hydrogenolysis of glycerol in liquid water over bifunctional supported Pt-Re nanoparticles. D. Falcone, J. Hack, A. Klushin, A. Knop-Gericke, R. Schlögl, **R.J. Davis***

13:25 – 97. Novel support materials for noble metal nanoparticle catalysts. **A.D. Quast***, M. Bornstein, I. Zharov, J.S. Shumaker-Parry

13:43 – 98. Advanced electron microscopy techniques for in situ liquid imaging of metal nanoparticles towards water-phase catalysis. **I. Arslan***, L. Parent, P. Abellan, T. Woehr, K. Jungjohann, G. Yang, J. Lercher

14:08 – 99. Hydrothermal conversion of biomass at supercritical conditions for gaseous fuel production: Results, new challenges, and developments. **C. De Blasio***, T. Kohl, M. Magdeldin, T. Westerlund, M. Järvinen

14:26 Break (15 min)

14:41 – 100. Bimetallic structure considerations in the catalytic production of aromatic amines. L.A. Pretzer*, K.N. Heck, J. Miller, **M.S. Wong**

15:06 – 101. Selectivity control of Au-catalyzed oxidation of glycerol in water. **Z. Yuan**, S. Liu, Z. Gao, **B. Xu***

15:24 – 102. Au-Pd alloyed single-atom-catalysts: A highly efficient catalyst for C-C and C-N coupling reactions in water. **T. Zhang**, **A. Wang**, L. ZHANG, W. WANG

15:49 – 103. Transformation of carbohydrates into polyols on metal catalysts using metallic powder and water as the hydrogen source. **Y. Hirano***, K. Sagata, Y. Kita

16:07 – 104. Critical role of water in catalytic CO oxidation over Au/TiO₂ catalysts. **L.C. Grabow***, H. Doan, J. Saavedra, C. Pursell, B. Chandler*

Hyatt Regency Waikiki
Mauka Blrm

Artificial Photosynthesis: Reduction of Carbon Dioxide (#271)

Organized by: O. Ishitani, E. Fujita, S. Kang
Presiding: H. Inoue, C.P. Kubiak

13:00 – 105. Reduction of CO₂ using photo-induced electrons and metal complexes bearing bases in the second coordination sphere and the alternative hydrogenation and hydride transfer reactions. **E. Fujita***, G. Manbeck, L. Duan, K. Garg, Y. Matsubara, J.T. Muckerman, Y. Hlimeda

13:25 – 106. Reactivity of metal-organic coordination networks for CO₂ activation. D. Hurtado Salinas, G. Ruano, K. Kern, **M. Lingenfelder**

13:40 – 107. Visible-light-driven photoconversion of carbon dioxide to formic acid using molecular metal catalysts and enzyme. **J. Kim**

14:05 – 108. Molecular architecture of supramolecular photocatalysts for CO₂ reduction in homogeneous and heterogeneous systems. **O. Ishitani**

14:30 – 109. Optimization of a dye/semiconductor/photocatalyst ternary system for carbon dioxide reduction. D. Won, J. Ji, **S. Kang***

14:55 Break

15:05 – 110. Monolithic semiconductor/metal-complex hybrid photocatalyst for solar CO₂ reduction coupled with H₂O oxidation. **T. Morikawa***, S. Sato, T. Arai, T.M. Suzuki

15:30 – 111. Photocatalytic reduction of carbon dioxide by carbon nitride with visible light. **K. Maeda***

15:55 – 112. Photocatalysts for the preferential reduction of carbon dioxide in the presence of water. S. Xie, Q. Zhang, **Y. Wang***

16:10 – 113. Photocatalytic and photoelectrochemical reduction of CO₂ using water as an electron donor. **A. Kudo***

16:35 – 114. Silver loaded titanate photocatalysts prepared by a flux method for reduction of carbon dioxide with water. **H. Yoshida***

Wednesday Morning

Hawaii Convention Center

Halls I, II, III

Chemistry of Automotive Emission Control Catalysts: Current R&D and Future Challenges (#21)

Organized by: C. Peden, D. Kim, M. Shen, W. Epling

Poster Session

10:00 – 12:00

11:5. Role of surface property of Rh/AlPO₄ catalyst in high tolerance to sulfur and phosphorous poisoning. **S. Minami**, H.P. Buwono, T. Hamada, Y. Hu, S. Hinokuma, H. Yoshida, M. Machida*

11:6. Selective catalytic reduction of NO with hydrocarbons: Effect of hydrogen and carbon monoxide addition for alumina catalyst. **A. Miyamoto***, N. Okazaki

11:7. Nature of Pd-Ru solid solution alloy nanoparticles for CO-oxidizing reaction. **H. Tomonaga**, K. Sato, T. Ishimoto, M. Koyama, T. Yamamoto, S. Matsumura, K. Kusuda, H. Kobayashi, H. Kitagawa, K. Nagao*

11:8. Oxygen storage capacity of FeNbO₄ synthesized by a polymerized complex method. **R. Maeda**, S. Hosokawa, K. Teramura, T. Tanaka

11:9. Preparation of highly dispersed Pd particles loaded on Al₂O₃ support for combustion of CO and C₃H₆. **T. Nakano**, K. Sato, K. Nagao*

12:0. Selective catalytic reduction of NO on transition-metal modified hexagonal Yb-FeO₃ catalysts. **T. Shibano***, S. Hosokawa, K. Teramura, T. Tanaka

Hyatt Regency Waikiki
Kou Ballrm

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli
Presiding: D. He, K.K. Pant, M. Uddin

8:00 Opening remark-Environmentally Friendly Chemical Production-II

8:02 – 121. Catalytic hydrogenation of carbon dioxide to methane with ammonia. **M. Uddin***, Y. Honda, H. Kakuta, Y. Nishimura, Y. Kato, K. Takagi

8:22 – 122. Manganese modified Fe₃O₄ microsphere catalyst with effective active phase of forming light olefins from syngas. **Y. Liu**, J. Chen, J. Bao, Y. Zhang*

8:42 – 123. Estimation of catalytic cracking reaction of model compounds using zeolite-containing hierarchical silica and silica-alumina catalysts by Curie point pyrolyzer. **A. Ishihara***, M. Ninomiya, H. Nasu, T. Hashimoto

9:02 – 124. Evaluation of basicity of layered double hydroxides (LDHs) by Knoevenagel condensations. **S. Yonekawa***, K. Teramura, S. Hosokawa, T. Tanaka

9:22 – 125. Selective production of acetol from glycerol on combustion synthesized and activated Cu-Al₂O₃ catalyst. **G.D. Yadav***, G.P. Fernandes

9:42 Break

* Principle Author

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9:57 Opening Remarks- Syngas and Biofuels-I
10:00 – 126. Nanostructured metal phosphide catalysts for conversion of biomass to liquid fuels. **S. Habas***, F. Baddour, D. Ruddy, C. Nash, M. Griffin, J. Hensley, J. Schaidle
10:20 – 127. CO₂ reforming of CH₄ to syngas over over Nd modified Ni/SBA-15 catalysts. H. Liu, **D. He**
10:40 – 128. Catalytic activity of heterogeneous base and acid catalysts for biodiesel production from green seed canola oil. **C. Baroi**, A. Dalai*
11:00 – 129. Oxidation of copper-exchanged small-pore zeolites and the active site for methane conversion. **B. Ipek***, M.J. Wulfers, J.P. Smith, K.S. Booksh, C. Brown, R.F. Lobo
11:20 – 130. Comparative study of noble metal impregnated Fe-Co bimetallic catalyst for the conversion of syngas to liquid fuel. . . **Sonal***, **K.K. Pant**, S. Upadhyayula
11:40 – 131. Selective dehydrocyclization of *n*-heptane using zeolite-alumina composite supported NiMo catalysts. **A. Ishihara***, A. Itoh, H. Nasu, T. Hashimoto

Hyatt Regency Waikiki
Ekahi

Progress Toward a Lignocellulosic Biorefinery (#144)

Organized by: A. Stipanovic, A. Varma, Y. Sung
Presiding: J.J. Bozell

8:00 – 132. New developments in lignocellulose, cellulose, and nanocellulose: Biofuels to bioproducts using advanced nanotechnology. **A.J. Varma***
8:40 – 133. Practical methyl levulinate synthesis from wood biomass using aluminumbased hybrid acid catalysts. **K. Tominaga***, K. Nemoto, A. Yamada, Y. Yamamoto, k. sato
9:00 – 134. Electrochemical functional group interconversions on biomass-derived compounds using nickel electrocatalysts in aqueous media. **J. van Drunen**, G. Tremilosi-Filho*
9:20 – 135. Seawater based biotechnology for biofuels and biomaterials production. **G. Chen***

9:40 – 136. Novel production of furfural from biomass based on hot water extracted pentoses. **C. Wood***, T.E. Amidon, B.M. Bujanovic

10:00 – 137. 5-(Chloromethyl)furfural (CMF) is the new HMF: Functionally equivalent but more practical in terms of its production from biomass. **M. Mascal***

10:20 – 138. Systematic investigation of chemical pretreatments for the enzymatic hydrolysis of Loblolly Pine wood. **L.A. Lucia***, R. Ghiladi, X. Du

10:40 – 139. Ultrasonic-assisted fractionation of bioproducts from oil palm fronds by alkaline pretreatment followed by simultaneous saccharification and fermentation. **K. Lee**, C. Ofori-Boateng*

11:00 – 140. 2G sugars to chemicals: Agri-industry of the future. **A. Lalí**

11:20 – 141. Pink pigmented facultative methylotrophic strain (PPFMs) isolated from plant phyllosphere for the production of cellulase. C. Molina, G. Hernandez, J. Gonzalez, I. Valdez-Vazquez, Y. Sanchez-Ruan, **G. de la Rosa**

Hyatt Regency Waikiki
Elma

Dynamical Processes of Light Harvesting Surfaces (#178)

Organized by: G. Thornton, M. Henderson, H. Onishi, C. Li, G. Herman
Presiding: C. Li, G. Thornton

8:00 Break

8:20 – 142. Excited state dynamics at complex interfaces: Time-domain ab initio studies. **O. Prezho**
8:50 – 143. Effect of TiO₂ crystal orientation on the adsorption and photoinduced electron transfer: CdSe quantum dot-sensitization system. **T. Toyoda***, w. Yindeesuk, K. Kamiyama, S. Hayase, Q. Shen
9:20 – 144. Ultrafast charge transfer dynamics in Au/quantum dot/molecular adsorbate tri-composite system. **H.N. Ghosh***
9:50 – 145. Exciton transport, dissociation, and light-driven H₂ generation in semiconductor-metal colloidal nanorod heterostructures. **T. Lian**
10:20 Break
10:30 – 146. Charge separation promoted with phase junctions and cocatalysts in photocatalysis systems. **C. Li***
11:00 – 147. Morphology and interface control for stable and reproducible perovskite solar cells. **Y. Wu**, X. Yang, W. Chen, Y. Yue, A. Islam, L. Han
11:15 – 148. Time-resolved visible to mid-IR absorption study on the behavior of photogenerated electrons and holes in LaTiO₃N visible light responsive water splitting photocatalysts. **A. Yamakata**, M. Kawaguchi, J. Kubota, K. Domen
11:30 – 149. Electron-hole recombination and surface reconstruction controlled by doping sites in Sr-doped NaTaO₃. **H. Onishi***

Hyatt Regency Waikiki
Maloko BlrM

Water-phase Catalysis for Energy and Chemicals Production (#182)

Organized by: M. Wong, C. Zhang, S. Jeong
Presiding: C. Sievers, Z. Zhang

8:00 – 150. Water-phase solar fuel and solar chemical production. **J. BAEG***
8:25 – 151. Effective catalytic cycle of CO₂ hydrogenation/formic acid dehydrogenation by Ir complex in water. **N. Onishi**, S. Xu, Y. Manaka, Y. Himeda*
8:43 – 152. Opportunities for aqueous phase catalysis in water management. **M.A. Reynolds***

9:08 Break (15 min)
9:23 – 153. Synergistic co-processing of red mud with pyrolysis bio-oil: From neutralization to catalysis. **M. Schlaf***, E. Karimi, C. Gissane, V. Jollet

9:48 – 154. Novel catalysts for selective reactions and simultaneous separation in biphasic systems. **D.E. Resasco***

10:13 – 155. Transformation of 5-HMF to fine chemicals via homogeneous catalysis in aqueous solution. Z. Xu, B. Chung, P. Yan, **Z. Zhang**, M. Schlaf

10:31 – 156. Evaluating heterogeneous catalyst stability in supercritical water. **J. Jocz**, P. Savage*, L. Thompson*

10:49 – 157. Aqueous-phase catalytic conversion of cellulose and xylose. **E. Park**

Hyatt Regency Waikiki
Mauka BlrM

Artificial Photosynthesis: Reduction of Carbon Dioxide (#271)

Organized by: O. Ishitani, E. Fujita, S. Kang
Presiding: M. Kanan, A. Kudo

8:00 – 158. Photocatalytic conversion of carbon dioxide to fuels using layered double hydroxide-based catalysts: Optimized performance and the reaction mechanism. **Y. Izumi**, N. Ahmed, M. Morikawa, S. Kawamura

8:25 – 159. Time and energy efficient synthesis and characterization of p-type semiconductor nanostructures for photoelectrochemical fuel generation. **C. Janaky***, D. Hursan, K. Rajeshwar

8:40 – 160. Photocatalytic and photoelectrochemical CO₂ reduction under solar light. **T. Ohno**

8:55 – 161. Inexpensive architectures for the production of fuels from carbon dioxide and sunlight. **J. Rosenthal***, J. DiMeglio, J. Medina-Ramos
9:20 – 162. Artificial photosynthesis: Photocatalytic conversion of CO₂ into renewable hydrocarbon fuel. **Y. Zhou***
9:35 – 163. Development of tailored heterojunction photocathodes for high efficiency artificial photosynthesis from CO₂ and water. **H. Park***
9:50 Break
10:00 – 164. Electrocatalytic CO₂ reduction to fuels and chemicals: Insights into transition metal surfaces. **T.F. Jaramillo***, K. Kuhl, T. Hatsuake, E. cave, D. Abram, C. Hahn, J. Feaster, A. Jonigerius, J. Kibsgaard
10:25 – 165. Hierarchical 3D Cu pillar and Sn dendrite as high performing electrocatalysts for CO₂ reduction. **S. Woo***, D. Won
10:40 – 166. Mechanistic insights into carbon dioxide reduction catalyzed by pure metal surfaces. **Y. Surendranath**, A. Wuttig
10:55 – 167. Photothermalchemical approach to reverse the alkane combustion reaction: CO₂ to C₅+ liquid hydrocarbons in one step. **F.M. MacDonell***, B. Dennis, W. Chanmanee, M.F. Islam
11:20 – 168. Selective and efficient electrochemical reduction of CO₂ on CuO-derived Cu nanowires. **W. Smith**
11:35 – 169. C-C bond-forming reactions to reduce CO₂ emissions. **M. Kanan***

Hawaii Convention Center
Halls I, II, III

Artificial Photosynthesis: Bio-inspired Chemistry for Solar Fuel Production (#278)

Organized by: H. Hashimoto, Y. Amao, J. Zhang, T. Moore, B. Koivisto
Presiding: Y. Amao, H. Hashimoto, B.D. Koivisto, T.A. Moore, J. Zhang

Poster Session 10:00 – 12:00

170. Visible light reduction of ketones and aldehydes catalyzed by complexes based on Earth abundant elements and water as source of hydrogen atoms. **A. Call**, F. Acuña-Páres, J. Lloret-Fillol

171. Constructions and characterizations of mutants containing bacteriochlorophyll *c*, *d*, *e*, or *f* of the green sulfur bacterium *Chlorobaculum limneum*. **J. Harada**, Y. Shibata, M. Ryono, M. Teramura, K. Yamamoto, T. Mizoguchi, H. Tamiaki

172. Studies on electrocatalytic CO₂ transformation by half-metallocene group 9 metal complexes. **W. Han***

173. Design of visible light driven photocatalyst with a sulfoalkarenane linker between zinc porphyrin and a Pt-TiO₂ for hydrogen evolution. **H. Imai**, T. Kamegawa, H. Yamashita*

174. Artificial light-harvesting antenna systems as models of chlorosomes using mesoporous silica. **T. Miyanya***, S. Shoji, Y. Goto, S. Inagaki, H. Tamiaki

175. Real time observation of vibrational wavepacket motions in ultrafast electron transfer systems. **Y. Nagasawa***, Y. Yoneda, S. Nambu, E. Takeuchi, H. Miyasaka

176. Observation of 8-vinyl-12-ethyl-bacteriochlorophyll-*e* in a green sulfur bacterium cultured by intense red-light illumination. **C. Okada***, T. Mizoguchi, J. Harada, H. Tamiaki

177. Construction of artificial light-harvesting devices using isolated chlorosomes from photosynthetic green bacteria. **M. Ryono**, J. Harada, Y. Tsukatani, T. Mizoguchi, H. Tamiaki*

178. Reconstitution of amphiphilic zinc bacteriochlorophyll *a* derivatives to major antenna complexes of green sulfur photosynthetic bacteria toward hybridization of natural photosynthetic light-harvesting systems with artificial energy acceptors. **Y. Saga***, N. Takahashi, T. Miyatake, H. Tamiaki

179. Photocatalytic carbon dioxide reduction from organic-inorganic hybrid system. **D. Won, J. Ji, H. Son***

180. Luminescent properties of copper(I) iodo coordination polymers containing two bridging amine ligands. **S. Sugimoto**, N. Ogawa, S. Yamashita, H. Ohtsu, K. Nozaki, K. Tsuge
181. Photochemical oxygenation reaction of cyclohexene sensitized by novel Ru(II) porphyrin/clay nanosheet complex. **D. Tatsumi**, T. Tsukamoto, T. Shimada, S. Takagi

182. In-vitro assay to clarify the substrate specificity of demethoxy-carboxylase involved in chlorosomal bacteriochlorophyll biosynthesis. **M. Teramura**, J. Harada, T. Mizoguchi, H. Tamiaki
183. Synthesis of chlorophyll derivatives possessing alkenyl groups at the peripheral positions and their photophysical properties. **H. Tamiaki**, T. Miyatake
184. Synthesis of 20-substituted chlorophyll derivatives as models of bacteriochlorophylls-*c/d* and their self-aggregation. **A. Wada**, H. Tamiaki
185. Energy transfer between subunits of dimeric photosystem II monitored by femtosecond transient absorption spectroscopy. **Y. Yoneda***, T. Katayama, Y. Nagasawa, H. Miyasaka, Y. Umeha

Hawaii Convention Center
Halls I, II, III

Chemistry of Clean Energy Conversion, Storage, and Production General Posters 10:00 – 12:00

186. Microstructures of hydrocarbon gas hydrates synthesized with and without promoters. **H. Ohno***, K. Mitsuhashi, A. Hachikubo, H. Shoji, H. Minami

187. On the mechanism of catalytic hydrogenation of thiophene on hydrogen transition metal oxides bronze. **H. Cheng***

188. Comparative study on reaction mechanism of the MXene electrodes in non-aqueous Li⁺ and Na⁺ electrolytes. **H. Inumua***, S. Kajiyama, R. Morita, K. Gotoh, M. Okubo, A. Yamada

189. Theoretical estimation of zinc isotope fractionation between mantle and core. **K. Asai**, M. Abe*, F. Moynier, Y. Zempo, M. Hada

190. Synthesis of organic dyes with benzimidazoles as electron transport chain for dye sensitive solar cell. **T. Iida**, M. Ota*, S. Ohata, H. Kajino

191. Synthesis and oxidative properties of ionic liquid-supported IBX. **A. Mihoya**, S. Koguchi

192. Anodic performances of electrodeposited Si films on structured Cu_xO_y surfaces for Li ion battery. **M. Matsunaga***, Y. Uchida, S. Kuno

193. Techno-economical evaluation of extractive fermentation by acetone, butanol, ethanol (ABE) production. **V.H. Grisales***, G. Olivari Tost

194. In vitro production of isoprenol using novel mevalonate pathway enzymes from thermoplasmic acidophilum. **M.C. Cummins**, J. Vinokur

195. Photocatalytic chemoselective reduction of epoxides to alkenes in alcoholic suspensions of silver-loaded titanium(IV) oxide at room temperature without use of reducing gas. **H. Kominami***, S. Yamamoto, I. Kazuya, A. Tanaka, K. Hashimoto

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- 196.** Preparation and thermoelectric properties of highly oriented CNT/elastomer composites. **T. Mashio**, M. Ota*, K. Kanai, M. Ikeda
- 197.** Binding mechanisms of cesium on clay minerals. **K. Baek***, J. Lee, E. Jeon, S. Ryu
- 198.** Fischer-Tropsch synthesis over iron catalyst supported on ozone treated active carbon. **Y. Kawahara**, K. Koimiyama, k. asami
- 199.** Preparation of silicon nanoparticles-containing porous carbon microspheres for lithium ion secondary battery anodes. **K. Arai**, M. Ota*, T. Ishibashi, M. Saitoh, N. Yoshizawa, K. Imoto, O. Tanaike, J. Miyawaki, y. Seong-Ho
- 200.** Iron anode-mediated activation of per-sulfate. **K. Baek***, P. Jeon, S. Park, S. Shin
- 201.** Synthesis of π -conjugated polarizable organic dyes with polycyclic aromatic ring as photosensitive group. **M. Tanaka**, M. Ota*, H. Kajino, T. Iida
- 202.** Effect of the kinds of metal in metal-filled CNT/C composites on thermoelectric properties. **K. Kanai**, M. Ota*, K. Suzuki, R. Matsumoto
- 203.** Deterioration behavior of Ni/TiO₂ catalyst for the selective CO methanation and its improvement method. **M. Fujiwara**, K. Tani, N. Shimoda, S. Satokawa
- 204.** Dye-sensitized solar cells based on TiGa treated TiO₂ photoactive electrodes. **j. yamakawa**, Y. Shimoyama, R. Tsubota, K. Tomita, Y. Kunugi
- 205.** Electrochemical reduction of carbon dioxide with EC tag (Cu) supported carbon electrode. **T. Namise**
- 206.** Upgrading of new hydrocarbon biodiesel fuel (HiBD). **H. Kuboyama**, Y. Murakami, H. Tani, k. asami, K. Fujimoto, T. Vilitdsant, P. Prasert Reubroycharoen, K. Wattanavichien
- 207.** Catalytic reforming of glycerin with iron ore. **m. yoshida**, k. asami, y. mogi, h. saima
- 208.** Effect of boron on electrostatic capacitance in electrodes for electric double layer capacitor. **S. Obokata**, M. Ota*, Y. Miyazawa, K. Suzuki, K. Arai
- 209.** Slurry phase synthesis of new hydrocarbon biodiesel fuel (HiBD). **T. Hirakawa**, H. Tani, Y. Murakami, K. Fujimoto, k. asami
- 210.** Naphthalo[2,1-b;3,4-b'dithiophene(NDT)-based bulk heterojunction organic solar cells. **H. Song**, Y. Kim, Y. Cheon, M. Kim, J. Baek, D. Chung, C. Park, Y. Kim*
- 211.** Impact of natural and artificial fluctuation in illumination intensity on the photo-synthetic activity of *Synechocystis* PCC 6803. **J. Kwon***
- 212.** Design and operation of selective CO oxidation reactor with a Ru/Al₂O₃ coated metallic structured catalysts for kW class PEMFCs application. **D. Seo***, W. Kim, Y. Hwang, W. Yoon
- 213.** Improvement of cathode catalyst layers for PEFCs by the electrostatic inkjet method. **K. Takahashi***, M. Watanabe, M. Uchida
- 214.** Hydration/dehydration reaction characteristics of natural calcium resources for chemical heat pump. **H. Ogura***, . Mitsui
- 215.** Recycle disposable heating pads as a visible light active photocatalyst. **C. Wang***, M. Lee, C. Chen, C. Wang*, . Hsiao, D. Tsai
- 216.** CNT supported Re catalyst for dimethyl ether direct-oxidation to dimethoxy dimethyl ether. **Q. Zhang**, W. Wang, Z. Zhang, Y. Tan*, Y. Han*
- 217.** Salting-out of acetone, 1-butanol, and ethanol from a prefractionator. **S. Xie**, C. Yi, X. Qiu, D. Yang
- 218.** Synthesis of N-defect and O-doping g-C₃N₄ and its visible light photocatalytic activity. **T. Mitsuyama**, H. Katsumata*, T. Suzuki, S. Kaneko
- 219.** Photocatalytic degradation of bisphenol A over bismuth oxydides. **T. Sasaki**, S. Kaneko, H. Katsumata*, T. Suzuki
- 220.** Production of nano carbon with direct alcohol reforming. **N. Hamaya***, N. Okazaki
- 221.** Direct methane reforming: Effect of the addition of silica. **A. Otsuka***, N. Okazaki
- 222.** Surface functionalization induced triboelectric charging sequence as a novel method to generate triboelectricity. S. Shin, m. lee, J. Nah*
- 223.** Comparative study on the sulfur tolerance of noble metal catalysts in methane steam reforming. **F. Watanabe**, I. Kaburaki, N. Shimoda, S. Satokawa*
- 224.** Development of nanostructural controlled silver phosphite thin films as a photo-anode for water splitting under visible-I. **H. Katsumata***, T. Hayashi, T. Suzuki, Y. Fujita, S. Kaneko
- 225.** Oxygen sorption/desorption properties of Sr-Ca-Fe-based perovskite oxides. **K. Izumihara**, A. TSUCHIDA, H. Ikeda, N. MIURA*
- 226.** Synthesis of biodiesel fuel from gutter oil. **G. Nakagawa**, S. Yodoya, Y. Sawada*
- 227.** Waste water treatment in biodiesel fuel process. **H. Kai**, D. Sugita, R. Watanabe, Y. Sawada*
- 228.** Synthesis of structurally-defined, sulfo-phenylated oligophenylenes, and poly-phenylenes for PEM fuel cells. **T. Skalski***, T.J. Peckham, S. Holdcroft
- 229.** Kinetics study on synthesis of biodiesel fuel. **O. Yan**, A. Kodama, Y. Sawada*
- 230.** Suppression of aluminum corrosion in highly concentrated electrolyte. **C. Chiang***, Y. Yamada, K. Sodeyama, J. Wang, Y. Tateyama, A. Yamada
- 231.** Chemical upgrading of low-rank coals by solvent treatment. **T. Takanohashi**, N. Sakimoto, Y. Harada, H. Fujimoto
- 232.** Influence of Cu on the performance of K-LaZrO₂ catalysts for isobutanol synthesis. Y. Wu, S. Wang, H. Xie, J. Gao, S. Tian, Y. Han, Y. Tan*
- 233.** Halogen-free borate ionic liquids for tribological applications. **M.K. McCray**, Z. Huang, D.M. Schubert
- 234.** Cycloaddition of CO₂ into epoxides over polymer supported ionic liquid catalysts. A. Jadhav*, R. Shavi, J. Seo*
- 235.** Detection of the intermediate species for oxygen evolution reaction on α -Fe₂O₃ using in-situ UV-vis absorption measurement. **K. Ishikawa**, T. Takashima, H. Irie*
- 236.** Performance of photofuel cells using aliphane-titania nanocomposite electrodes. **H. Nishikiori**, N. Furuchi
- 237.** New cathode of high capacity and superior cyclability for Na-ion batteries: Na_{0.6}Fe_{0.2}Mn_{0.4}xTi_{0.2}O₂. **X. Sun**
- 238.** Life-prolonging technique of lubrication oil by continuously regenerating anti-oxidant with catalytic palladium membrane. **N. Itoh***, K. Ohshima, T. Sato, J. Shinoda, M. Kobesho
- Wednesday Afternoon**
- Hyatt Regency Waikiki
Elma
- Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)**
- Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli
Presiding: N. Braidy, A. Dalai
- 13:00** Opening Remarks-Syngas and Biofuels-II
- 13:02 – 239.** Performance and nanostructural analysis of a novel nickel alumina catalyst for dry reforming of methane. **N. Braidy***, J. Blanchard, N. Abatzoglou
- 13:22 – 240.** Preparation of H- β zeolite–enwrapped Co/Al₂O₃ Fisher-Tropsch catalyst for high isoparaffins selectivity. **H.L. Nguyen**, Y. Yoneyama*, N. Tsubaki
- 13:42 – 241.** Spontaneously activatable iron-based Fischer-Tropsch catalysts. **D. Chun***, G. Rhim, J. Park, H. Lee, J. Yang, S. Hong, H. Jung
- 14:02 – 242.** Syngas hydrogenation: Effect of preparation variables on the performance of cobalt-nickel catalyst. **K. Ramasamy**, M. Gray, H. Job, y. wang
- 14:22 – 243.** Effect of preparation condition change of Ni/Al₂O₃ structured catalyst on CO₂ dry-reforming performance. **T. Osuka**, Y. Kohno, R. Watanabe, C. Fukuhara
- 14:42 Break**
- 14:57** Opening Remarks-Syngas and Biofuels-III
- 15:00 – 244.** Doping effect of trivalent cation on the catalytic behavior and properties of Co-Ni-Mg-O solid solution catalysts in syngas production by methane reforming under high pressure. **K. Nagaoka***, Q. Han, G. Kitayama, T. Ishikawa, Y. Abe, Y. Hashimoto, K. Sato, Y. Takita, T. Wakatsuki, M. Kunisu, E. Suda, S. Inamoto
- 15:20 – 245.** Hydrothermal synthesis of structure-type iron oxide catalyst for water gas shift reaction. **R. Watanabe**, S. Watanabe, C. Fukuhara
- 15:40 – 246.** Selectivity control for CO methanation in hydrogen-rich gas containing a large amount of CO₂ over Ni/Al₂O₃ catalysts by vanadium addition. R. Inoue, T. Miyao, K. Higashiyama*, M. Watanabe
- 16:00 – 247.** Hydrodeoxygenation of palm oil to biofuel over Ni₂P/MOR in a trickle bed reactor. J. Wittayakun, S. Rakmae, N. Viriya-empikal, K. Faungnawakij, P. Hemthong*
- 16:20 – 248.** Oxorhenium catalyzed deoxydehydration for the diols and biomass derived polyols to alkenes and value added chemicals. **I. Ahmad***, S. Waseem
- Hyatt Regency Waikiki
Ekahi
- Theory and Computation for Efficient Utilization of Energy and Resources (#163)**
- Organized by: Q. Ge, W. Li, H. Cheng
Presiding: W. Li, J. Yang
- 13:00 – 249.** Transition metal atom embedded graphene for capturing CO: A first-principles study. **J. Yang**
- 13:35 – 250.** Size-dependent catalytic properties over metal nanoparticles: Simulation and experiment. **J. Wang***
- 14:05 – 251.** Reduction and hydrogenation of CO₂ over In₂O₃-based catalysts. **Q. Ge**, J. Ye, C. Liu
- 14:35 – 252.** Theoretical design new mixed solids for CO₂ capture applications. **Y. Duan***
- 14:55 Break**
- 15:05 – 253.** Structure-energy-activity relations in heterogeneous catalysis. **P. Sautet**, F. Calle Vallejo, D. Loffreda
- 15:40 – 254.** First-principles calculation on syngas conversion. **W. Li***
- 16:10 – 255.** Stochastic simulation: Understanding the CO activation mechanisms in Fischer-Tropsch synthesis on Fe(110) model surfaces. Z. Chen, H. Wang, X. Xu
- 16:40 – 256.** On the mechanism of CO₂ reduction to methanol on CeO₂(110) surface. **M. Haider***, N. Kumari, N. Sinha, S. Basu
- Hyatt Regency Waikiki
Maloko Blrm
- Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188)**
- Organized by: K. Miyatake, M. Tada, Y. Sung, B. Pivovar, M. Hickner
Presiding: K. Miyatake, S.J. Paddison
- 13:00** Opening remark
- 13:05 – 257.** Structural aspects of PFSA ionomers as determined by STEM and simulations. **S.J. Paddison***
- 13:45 – 258.** Evaluation of CeO₂, ZrO₂ and YSZ as degradation-mitigating additives for proton electrolyte membrane fuel cells. **T. Weissbach**, T.J. Peckham, S. Holdcroft*
- 14:05 – 259.** Electronically stabilized, high-performance PEMs as fully hydrocarbon fuel cells. **B.D. Britton**, H. Lee, W. Huang, S. Holdcroft*
- 14:25 – 260.** Synthesis of polyphenylene-based polymer electrolytes by catalyst transfer polycondensation (XII): Mass transport characteristics. **T. Oshima**, H. Takagi, M. Fujita, A. Ohira, Y. Takeoka, M. Rikukawa
- 14:45 – 261.** Theory of polymer electrolyte membranes: Cradle to grave. **M. Eikerling**
- 15:25 – 262.** Effect of the interfacial structure of proton conducting ionomers on the fuel cell performance. **T. Mochizuki**, J. Miyake, M. Uchida, H. Uchida, K. Miyatake*
- 15:45 – 263.** Homogeneous coating of ionomers on electrocatalyst assisted by polybenzimidazole as an adhesive layer and its effect on fuel cell performance. **T. Fujigaya**, Z. Yang, N. Nakashima
- 16:05 – 264.** Proton transport property at Nafion-Pt interface. **Y. Ono**, Y. Nagao*
- 16:25 – 265.** Novel hydrocarbon ion-conducting polymers for proton exchange and anion exchange fuel cell membranes. **C. Bae***
- Hyatt Regency Waikiki
Makai Blrm
- New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250)**
- Organized by: Y. Yang, S. Meng, A. Yamada, Y. Sun
- 13:00 – 266.** Pseudocapacitance of MXene Ti₂CT_x nanosheets for high power sodium-ion hybrid capacitors. **M. Okubo***, X. Wang, S. Kajiyama, H. Inuma, S. Oro, I. Moriguchi, A. Yamada
- 13:15 – 267.** Implications and performance of various lithium ion battery chemistries during high precision coulometry. **A. Masias***, J. Marcicki, T. Coupar
- 13:30 – 268.** Feasibility of stainless steels as current-collectors in high-performance lithium-ion batteries. **M. Morita***, M. Araki, K. Fujii, N. Yoshimoto
- 13:45 – 269.** Effect of porous structure of carbon substrates for sulfur composite cathode on performance of Li-S batteries. **A. Ikoma***, S. Zhang, K. Ueno, K. Dokko, M. Watanabe
- 14:00 – 270.** Thin nanosheet Li₂FeP₂O₇ cathode for high energy Li-ion battery. **D. S***
- 14:15 Break**
- 14:30 – 271.** Design of photoelectrode system for oxidative production of hydrogen peroxide in water splitting. **K. Fuku**, K. Sayama*
- 14:45 – 272.** High efficiency planar heterojunction solar cells based on perovskite fabricated with two-step solution process. **C. Wu**
- 15:00 – 273.** A peek at electrolyte-cathode interactions. **S.M. Russell**, A.v. Cresce, K. Xu
- 15:15 – 274.** Low molecular weight cyclic organoboron electrolytes for Li ion batteries. **P. Joshi***, R. Vedarajan, N. Matsumi
- 15:30 – 275.** Effects of additive components on the electrochemistry of Mg(TFSAs)/triglyme electrolyte for rechargeable magnesium batteries. **N. Yoshimoto***, I. kim, T. Kimura, K. Fujii, M. Morita

* Principle Author

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<http://pacificchem.org/onlineprogram>

15:45 – 276. In-situ characterization of tetrahydrofuran containing Grignard reagents in magnesium deposition and dissolution processes. **H. Inoue**, Y. Akitा, H. Munakata, K. Kanamura*

Hyatt Regency Waikiki
Kou Ballrm

Artificial Photosynthesis: Bio-inspired Chemistry for Solar Fuel Production (#278)

Organized by: H. Hashimoto, Y. Amao, J. Zhang, T. Moore, B. Koivisto
Presiding: Y. Amao, H. Hashimoto, O. Ishitani, B.D. Koivisto, T.A. Moore, J. Zhang

13:00 – 277. Theoretical study of highly efficient CO₂ capturing processes using tricarbonyl diimine transition metal complexes. **J. Maeba**, M. Iwamura, K. Nozaki

13:15 – 278. Utilization of FTIR-ATR spectroelectrochemistry to evaluate the mechanism of aqueous CO₂ reduction on post-transition metal electrodes during CO₂ reduction. **J.E. Pander***, M.F. Baruch, A.B. Bocarsly

13:30 – 279. Photoelectrochemical CO₂ reduction using Ru(II)-Re(I) metal complex on semiconductor electrodes. G. Sahara, **H. Kumagai**, R. Abe, T. Morikawa, K. Maeda, O. Ishitani*

13:45 – 280. Role of surface-bound carbonates in the reduction of CO₂ on tin cathodes. **M.F. Baruch***, J.E. Pander, J.L. White, A.B. Bocarsly

14:00 – 281. Electrochemical reduction of CO₂ by Ni cyclam complex substituted with imidazole type ionic liquid. **T. Nagai***, A. Katayama, T. Ozawa, T. Inomata, H. Masuda

14:15 – 282. Development of metal sulfide photocathodes with chalcocite structure for CO₂ reduction under visible light irradiation. **T. TAKAYAMA**, A. Iwase, A. Kudo

14:30 Break & Opening Remark for AP03 session

14:45 – 283. Strategies to enhance the light harvesting capacity of artificial light harvesting nano structures. **R. Cogdell***

15:15 – 284. Artificial light-harvesting antenna systems using self-assemblies of semi-synthetic chlorophylls. **H. Tamiaki***, S. Shoji

15:30 – 285. Molecular mechanism of action of the cyanobacterial orange carotenoid protein. **R.E. Blankenship***, H. Liu, J. King, H. Zhang, D. Niedzwiedzki, M.L. Gross

16:00 – 286. Photoinduced charge separation processes: From natural photosynthesis to organic photovoltaics. **O. Poluektov***

16:15 – 287. Artificial light harvesting model by a hexameric hemoprotein reconstituted with zinc porphyrinoid. **T. Hayashi***, T. Mashima, K. Ooshora

Hyatt Regency Waikiki
Mauka Blrm

Homogeneous Catalysis Methodologies for the Upgrading of Biomass Derived Molecules (#301)

Organized by: J. Gordon, R. Baker, T. Ikariya
Presiding: J. Gordon

13:00 – 288. Acid-, water- and high temperature-stable homogeneous catalysts for the hydrodeoxygenation of biomass derived sugars and sugar condensates to value-added alcohols, alkenes, and alkanes. **M. Schlaf**, R. Sullivan, E. Latifi, B.K. Chung, D. Soldatov

13:35 – 289. Challenges and opportunities in the selective transformation of biomass to chemical intermediates and materials. **R. Waymouth***

14:10 break

14:20 – 290. Homogeneous catalysis of hydrogenation and hydrogenolysis reactions. **K. Goldberg**

14:45 – 291. New catalytic reactions and catalysts for the deoxygenation of carbohydrates. **A.D. Sadow***

15:10 break

15:20 – 292. Sulfuric acid as a catalyst for ring-opening of biobased bis-epoxides. **G.B. Bantchev***, K.M. Doll, G. Biresaw, K.E. Vermillion

15:45 – 293. Selective flow epoxidation and epoxide ring-opening of biorenewable terpenes for chemical manufacture. **W. Cunningham***, M. Hutchby, S.D. Bull, m. davidson

16:10 – 294. Catalytic conversion of biomass by transforming lignin first into aromatic fuels and chemicals. **M.M. Abu-Omar***

16:35 – 295. Adding value to biomass: Green gold! **A. Sutton**, J. Gordon, P. Silks, R. Wu

Wednesday Evening

Hyatt Regency Waikiki
Kou Ballrm

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli

Presiding: A. Dalai, Y. Hu

19:00 Opening Remarks-Nanocatalysis- Structural Study-I

19:02 – 296. In situ X-ray absorption spectroscopy studies of Fe nanoprecursors and Fe@Fe_xPd nanocatalysts. Y. Yao, A. Maclellan, **Y. Hu***, R. Scott*

19:22 – 297. Investigation of NH₃ poisoning mechanism and doping effect of Pt for CO preferential oxidation catalyst with using *in-situ* XAFS analysis. **K. Sato**, S. Zaitsu, K. Teramura, T. Tanaka, K. Nagaoka*

19:42 – 298. Characterization of a novel Ni/YSZ catalyst with strong tolerance to coke deposition for direct internal reforming (DIR) - SOFC. **W. Kawasaki**, Y. Kohno, R. Watanabe, C. Fukuhara

20:00 – 299. In-situ XAS monitoring the formation and the electrochemical behaviors of nanomaterials for energy applications. **C. Kongmark***, N. Kochaput, P. Khemthong, S. Sangsawan, P. Viravathanava, V. Somsongkul, M. Arunchariya

20:20 – 300. DFT investigation of the Mo₃S_xH_y ($x=5-9, y=0,2,4$) clusters and their role in hydrodesulfurization catalysis. **J.D. Head***, C. Tanabe, K. Gotto, J. Siu, M. Mallory

20:40 – 301. Finite size effects in sub-monolayer catalysts. **L.C. Grabow***, H. Doan, Q. Yuan, S. Brankovic*

Hawaii Convention Center
Halls I, II, III

Progress Toward a Lignocellulosic Biorefinery (#144)

Organized by: A. Stipanovic, A. Varma, Y. Sung

Poster Session

19:00 – 21:00

302. Chemical and morphological characterization of depithed bagasse for the purpose of gasification using computer simulation. **A.I. Anukam***, S. Mamphweli, P. Reddy, E. Meyer, O. Okoh

303. Novel method to convert paper mill waste into valuable fermentable sugar. **B. Bhayani**

304. Improving levoglucosan synthesis from pyrolysis of functionalized glucose. **L. Chen***, J. Zhao, S. Pradhan, B.E. Brinson, G. Scuseria, Z. Zhang, M.S. Wong

305. Catalytic fast pyrolysis of biorefinery lignins for the production of low molecular weight phenolic compounds. **D.B. Corbett***, O. mante, B.M. Bujanovic

306. Increasing the value of the biorefinery: Lignin-furfural based novel green wood adhesives. **P.S. Dongre***, M. Driscoll, J. Smith, T.E. Amidon, B.M. Bujanovic

307. Characterization of amphiphilic lignin from cattle fecal as an emulsifier. **T. Fujiwara***, K. Iwabata, Y. Kanai, T. Ruike, Y. Seki, K. Sakai, H. Sakai, K. Sakaguchi, M. Abe

308. Direct production of L-malic acid from lignocellulose by consolidated bioprocessing with *Schizophyllum commune*. **K. Hoshino***, M. Takano, E. Nagane, M. Hatashita

309. Microscopic observation of morphological changes in woody biomass as treated with ionic liquid. **T. Kanbayashi**, H. Miyafuji

310. Mass transfer characteristics of cellulose during hydrothermal treatment. **H. Kawasaki**, Y. Matsumura*

311. Catalytic depolymerization of lignin using self-generated active hydrogen from supercritical ethanol. s. jeong, G. Jang, Y. Park, D. Kim

312. Lignin-based polyoxyethylene ether enhanced enzymatic hydrolysis of cellulose and lignocellulose by dispersing cellulose aggregates. **H. Lou***, X. Lin*, X. Qiu*

313. Properties and regeneration of tertiary amines used in the recovery of acetic acid from kraft-based dissolving pulp process prehydrolysis liquors. G. Yang*, **L. Lucia**, Z. Zhang, J. Chen, Y. Ni

314. Properties and regeneration of tertiary amine from recovery of acetic acid from prehydrolysis liquors produced by the kraft dissolving pulp process. **L.A. Lucia**, G. Yang, Q. Jiang, J. Chen, Y. Ni

315. Preparation and analysis of Chaga mushroom (*Inonotus obliquus*) extracts for antioxidant activity and free phenolic hydroxyl group content. **A. Nagarolekar***, B.M. Bujanovic

316. Decomposition behavior of hemicelluloses in rice straw and rice husk as treated by hot-compressed water. **Y. Nakahara***, E. Minami, H. Kawamoto, S. Saka

317. Elucidation of the biolol properties produced by the developing Auger-type movable reactor. **S. Nishimura**, K. Ebihara*

318. Expression and characterization for cellulose degradation of the polysaccharide monoxygense from *Coprinopsis cinerea*. **K. Seino***, K. Iwabata, Y. Kanai, T. Ruike, Y. Seki, K. Sakai, H. Sakai, K. Sakaguchi, M. Abe

319. Bioethanol production from CaCO₃-removed paper sludge by thermotolerant fermenting-fungus. **M. Takano**, K. Hoshino*

320. One-pot high-gravity bioethanol fermentation from choline-based ionic liquid pretreated corn stover. **F. Xu**

321. Structural characterization of solubilized noncarbohydrate compounds during acidic water flowthrough pretreatment of Poplar wood. **L. Yan**

322. Degradation products from lignocelluloses as treated with ionic liquid-water mixtures. **K. Yoshioka***, H. Miyafuji, H. Ohno, T. Yamada

Hawaii Convention Center
Halls I, II, III

Water-phase Catalysis for Energy and Chemicals Production (#182)

Organized by: M. Wong, C. Zhang, S. Jeong

Poster Session

19:00 – 21:00

323. Photocatalytic hydrogen evolution from glycerol aqueous solution.

Y. Mizukoshi*, H. Nakanishi, F. Hori, K. Okitsu, A. Iwase, Y. Maeda, N. Masahashi

Hawaii Convention Center
Halls I, II, III

Current Status and Future Prospect of Polymer Electrolyte Cells (#188)

Organized by: K. Miyatake, M. Tada, Y. Sung, B. Pivovar, M. Hickner

Presiding: K. Miyatake, B. Pivovar, Y. Sung, M. Tada

Poster Session

19:00 – 21:00

324. Development of organic/inorganic hybrid PEMs functionalized gradient for PEFs fabricated by EB grafting and sol-gel method. **t. takura**, A. Oshima, M. Washio

325. Effect of ketone vs sulfone groups on the properties of Poly(arylene ether)-based proton exchange membranes. H. Lee, Y. Huang, B.D. Britton, T.J. Peckham, S. Holdcroft, **W. Huang**

326. Ladder-type aromatic block copolymers containing triphenylphosphine oxide moiety as proton conductive membranes. **Y. Zhang**, F. Hartanti, J. Miyake, M. Watanabe, K. Miyatake

327. Synthesis and properties of poly(phenylene)-poly(ether ketone) block copolymer electrolytes (V): Relationship between microstructure and ion exchange capacity. **S. Nagaya**, M. Fujita, Y. Takeoka, M. Rikukawa

328. Controlled synthesis of hydrophilic-hydrophobic diblock copolymers using two types of chain-growth polymerizations (I) - bifunctional initiator. **Y. Hoshikawa**, K. Ogu, M. Fujita, Y. Takeoka, M. Rikukawa

329. Synthesis and evaluation of graft-type hydrocarbon polymer electrolytes (III): Effect of graft density. **R. Ide**, M. Rikukawa, M. Fujita, Y. Takeoka

330. Synthesis of hydrocarbon ionomers and evaluation of MEA (V): Relationship between block chain length and electrochemically active surface area. **S. Miyata***, M. Fujita, Y. Takeoka, M. Rikukawa

331. Highly dispersed Pt NPs supported selectively on carbon black as effective cathode catalyst for polymer electrolyte fuel cells. **S. Yokoyama***, K. Motomiya, S. Tsuchida, T. Kojima, Y. Taniguchi, T. Hiramatsu, Y. Ueyama, M. Morita, H. Takahashi, K. Tohji

332. Improvement of barrier property of fuel cell membrane via layer by layer assembly and chemical modification. **C. Cho***

333. Electrocatalytic activity for oxygen reduction reaction of electrochemically constructed Ni-core Pt-shell nanoparticles. N. Aoki, T. Kondo*, M. Hirota, S. Shibata, A. Omachi, **M. Ueda**

334. Iron and copper co-doped oxygen reduction reaction catalysts. **T. Murotani**, M. Kato, I. Yagi*

335. Novel synthesis of Pt/rPGO by a pyrolysis method of graphene oxide and ORR property. **H. Hayashi**, K. Teramura, S. Hosokawa, T. Tanaka

336. Scale-up of Pd-Pt core-shell catalysts: Synthesis, characterization, and performance. **L. Yang**, D. Barham, S. Ye, S. Knights, E. Gyenge

337. In-situ time-resolved XAFS study on the degradation processes of Pt/C and Pt₃Co/C cathode catalysts in polymer electrolyte fuel cell by feed gas exchange cycles. **K. Higashi**, G. Samjeské, S. Takao, S. Nagamatsu, K. Nagasawa, O. Sekizawa, T. Kaneko, T. Uruga, Y. Iwasawa*

*** Principle Author**

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- 338.** In-situ time-resolved XAFS study on the kinetic behavior of PEFC Pt/C (Ketjen-black, acetylene black, CNT) cathode catalysts in potential-jump transient response processes. **T. Kaneko***, K. Nagasawa, S. Takao, K. Higashi, S. Nagarmatsu, G. Samjeske, O. Sekizawa, T. Uruga, Y. Iwasawa
- 339.** Investigation of cathode catalyst degradation under hydrogen passivation start-up and shut-down process for fuel cell vehicle. **Y. Yamashita**, S. Itami, T. Eguchi, J. Takano, M. Kodama, K. Kakimura, M. Hara, H. Uchida, M. Watanabe, M. Uchida*

Hawaii Convention Center
Halls I, II, III

Artificial Photosynthesis: Reduction of Carbon Dioxide (#271)

Organized by: O. Ishitani, E. Fujita, S. Kang

Poster Session
19:00 – 21:00

- 340.** Surface investigation of supported metal cluster catalysis for solar fuel synthesis. **G. Laufersky***, T. Nann, G. Andersson
- 341.** Photons to formate: Solar driven conversion of CO₂ to solar fuels. **H. Pan***, M. Heagy
- 342.** Novel microchannel reactor with fused glass beads waveguide for photocatalytic reaction. **H. Usami***, K. Ohta
- 343.** Novel photoreduction systems of CO₂ based on various arylane compounds. **E. Sakuda***, N. Ishizaki, M. Tanaka, S. Horiuchi, Y. Arikawa, K. Umakoshi, N. Kitamura*
- 344.** Ru(II)-Re(I) supramolecular photocatalysts for efficient CO₂ reduction in water. **A. Nakada***, K. Koike, K. Maeda, O. Ishitani

- 345.** Light induced CO₂ reduction on *p*-type semiconductor by zinc porphyrin and rhodium complex hybrid system. **D. Yamamoto**, Y. Ko, P.V. Nair, Y. Nabetai, H. Tachibana, H. Inoue*

- 346.** Effect of composition between SrTiO₃ photocatalyst and carbon dioxide adsorbent. **M. SAKAI***, T. Itai, V. Kalousek, N. Toshima, K. Ikeye
- 347.** Acceleration of electrocatalytic CO₂ reduction by adding PCET-inducing compounds. **T. Suzuki**, T. Takashima, H. Irie

- 348.** Improvement of photocatalytic activity of hybrids with ruthenium complexes and carbon nitride for CO₂ reduction under visible light. **R. Kuriki***, O. Ishitani, K. Maeda
- 349.** CO₂ reduction catalysts composed of modified cycloazalkenes. **M.A. Habib***, B.K. Breedlove, M. Yamashita

- 350.** Photocatalytic decomposition of CO₂ by layered double hydroxides. **K. Katsunata**, N. Matsushita, K. Okada

- 351.** Photoelectrochemical reduction of carbon dioxide utilizing boron-doped g-C₃N₄ loaded with co-catalyst (Au, Ag, Rh). **N. Sagara**, S. Kamimura, T. Ohno*

- 352.** Efficient photocatalytic CO₂ reduction system using rhodium complex intercalated into zirconium phosphate layered matrix. **M. Wen**, Y. Kuwahara, K. Mori, H. Yamashita*
- 353.** Highly efficient, selective, and durable photocatalytic system for erudition of CO₂ to formic acid. **Y. Tamaki**, O. Ishitani*

- 354.** Fabrication of co-catalyst loaded p-type Cu₄Nb₂O₈ photocathode toward photoelectrochemical reduction of carbon dioxide. **S. Kamimura***, T. Ohno

- 355.** Photocatalytic reduction of CO₂ with H₂O on 3D ordered macroporous TiO₂-supported core-shell noble metal@CdS nanoparticles. **J. jiao***, Y. Wei*, Z. Zhao*, J. Liu, A. Duan, J. Li, G. Jiang
- 356.** Electrochemical reduction of low concentration of CO₂ using Re(I) complexes as catalysts. **T. Nishikawa***, G. Sahara, Y. Tamaki, O. Ishitani

- 357.** Photocatalytic reduction of CO₂ using Mn(I) diimine carbonyl complexes with various substituents. **H. Kamiyama**, H. Takeda, O. Ishitani*
- 358.** Photocatalytic reduction of CO₂ over intercalated nanocomposites based on layered double hydroxides. **H. Jiang***, K. Katsumata*, N. Matsushita
- 359.** Photocatalytic CO₂ conversion into CO in H₂O over layered double hydroxide containing transition metal ions. **Y. Hasegawa**, K. Teramura, S. Hosokawa, T. Tanaka
- 360.** Photocatalytic conversion of CO₂ by H₂O over the rare-earth oxide-modified Ga₂O₃. **H. Tatsumi***, K. Teramura, S. Hosokawa, T. Tanaka
- 361.** Investigation of photoelectrochemical property of ZnGa₂O₄-modified Ga₂O₃ for photocatalytic conversion of CO₂ by H₂O. **S. Kikkawa***, K. Teramura, S. Hosokawa, T. Tanaka
- 362.** Syntheses of meso-substituted iron porphyrin complexes and analyses of photoreaction by photoelectrochemical measurement. **Y. Okabe**, A. Fukatsu, M. Kondo, S. Masaoka*
- 363.** A role of the Ag cocatalyst in the photocatalytic CO₂ reduction with water over Ga₂O₃. **M. Yamamoto**, T. Yoshida, N. Yamamoto, T. Nomoto, S. Yagi

- 364.** Investigating the interactions of CO₂ with photocatalytic nanomaterial surfaces. **L.M. Reyes**, L. Hoch, T.E. Wood, G. Ozin*
- 365.** Synthesis and characterization of copper(I) complexes having NAD model ligands. **M. Takaoka**, H. Ohtsu*, K. Tsuge, K. Tanaka*
- 366.** Photocatalytic CO₂ reduction by *trans*-[Cl]-Ru(bpy)(CO)₂Cl₂: A new mechanism for CO/HCOO⁻ selectivity. **H. Ishida***, J. Itabashi, K. Kitamura, Y. Kuramochi
- 367.** Simultaneous production of aniline and acetone, ethanol, and butanol (ABE). **V.H. Grisales**, G. Olivari Tost

Thursday Morning

Hawaii Convention Center
Halls I, II, III

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli

Presiding: S. Badoga, N. Mahinpey

Poster Session

10:00 – 12:00

- 368.** Synthesis and catalytic activities of multimetallic clusters using a dendrimer template. **H. Koizumi***, M. Takahashi, T. Imaoka, K. Yamamoto
- 369.** Preparation of copper-cobalt oxides catalyst for complete oxidation of low concentration benzene vapor at low temperature. **T. Kiso***, M. Uddin, Y. Kato
- 370.** Catalytic upgrading of furfural over ZSM-5 and metal/ZSM-5 catalyst: Effect of catalyst particle size and metal type. **K. Lee***, J. Lee, I. Lee, K. Hwang, J. Lee, J. Han
- 371.** Effect of active carbon loading amount on the performance of microcapsule encapsulated with CaO catalyst and active carbon powders for the methanolysis of rapeseed oil under the light irradiation. **R. Kadota***, T. Furusawa, F. Kurayama, M. Sato, N. Suzuki
- 372.** Hydrogenation of unsaturated organic molecules over a mesoporous Mo₃O₈ catalyst. **S. Fei**, P. Mei, H. Yan, **H. Cheng***
- 373.** Preparation of perovskite oxides by the hydrothermal synthesis method and their electrocatalytic activities for oxygen reduction reaction. **M. Kono***, Y. Miyahara, K. Miyazaki, T. Fukutsuka, T. Abe, M. Kawaguchi
- 374.** Preparation of metal catalyst-liposome complex for oxidation reaction. **Y. Takahashi**, K. Deguchi, T. Shimanouchi, Y. Kimura
- 375.** Oxidative dehydrogenation of 1-butene using copper ferrite catalyst prepared with activated carbon. **T. Kiyokawa***, N. Ikenaga
- 376.** Synthesis of 1,3-butadiene from ethanol with MgO-loaded Al₂O₃-ZrO₂ catalyst. **R. Fujibayashi***, N. Ikenaga
- 377.** Effect of iron addition on oxidative dehydrogenation of 1-butene using V-Mg complex oxide. **J. Hatayama***, N. Ikenaga
- 378.** One-pot synthesis of catalytic Rh nanocrystals encapsulated in carbon spheres for higher alcohol synthesis. **K. Ha***, J. Lim, D. Kim, H. Park
- 379.** Effect of mesoporous silica coating on catalytic activity of Ni/Al₂O₃ for selective CO methanation. **T. Kuroda**, T. Miyao, K. Higashiyama*, M. Watanabe
- 380.** Synthesis of Co-B-Ni/P core-shell nanoparticles for rapid hydrogen generation. **Y. Zou***, C. Xiang
- 381.** Physicochemical and catalytic properties of spherical Al₂O₃/porous coordination polymer(PCP) core/shell composites. **N. Kageura**, N. Ito, Y. Takeisi, K. Sato, K. Nagaoka*
- 382.** Application of immiscible palladium-ruthenium solid solution alloys to organic conversions. **H. Yamamoto**, K. Imamura, K. Sato, K. Kusuda, H. Kobayashi, H. Kitagawa, K. Nagaoka*
- 383.** Structural and electronic state analysis of visible light response Au loaded TiO₂ photocatalysts. **Y. MISU***, T. Yoshida, T. Sawai, J. Kumagai, S. Ogawa, S. Yagi
- 384.** Effect of carbon dioxide addition on Fischer-Tropsch synthesis using Fe-based catalyst. **T. Okawara**, T. Yoshida, Y. Yoneyama*, N. Tsubaki, K. Tanaka, Y. Shibata, M. Murata, T. Ishiyama, H. Higashimura
- 385.** Carbon dioxide electrolysis with EC tag (Ag) supported carbon electrode. **M. Morimoto**, T. Katsujii, T. Haruyama
- 386.** Glycerol electro-oxidation: Tuning selectivity by controlling diffusion of reactants and products to and from catalyst centre. **L. Thia***
- 387.** Ethylene oligomerization catalyzed by phenylsilane-modified zirconia. **Y. Imizu***, T. Nishiharaguchi, S. Kobayashi, H. Morikawa, H. Yamada
- 388.** Aromatization of light hydrocarbons over binary metal oxide/MFI zeolite under CO₂. **Y. Choi**, Y. Mo, S. Park*
- 389.** Side-chain alkylation of toluene with methanol over hierarchical zeolite under CO₂. **D. Seo**, N. Jiang, S. Park*
- 390.** Nanocast mesoporous alumina as solid acids for Friedel-Crafts reaction. **H. Choi**, J. Kim, S. Park*
- 391.** Synthesis and characterization of platinum-functionalized steel balls, and their thermal performance in a radio-frequency inductive heating system. **M.A. Laban***, D. Hayes, D. Boldor
- 392.** Synthesis, characterization, and catalytic evaluation of Ni-Mo/TiO₂ and Ni-V/TiO₂: Hydrodeoxygenation of guaiacol. **L. Katta, A. Aqsha, N. Mahinpey***
- 393.** Hydrothermal synthesis of face-centered cubic platinum-ruthenium core-shell and alloy nanocrystals with high electrocatalytic activity. **J. Gu**, Y. Guo, Y. Zhang
- 394.** Steam reforming of propane at low temperature over supported Rh catalysts. **L. Yu, K. Sato, Y. Sato, K. Nagaoka***
- 395.** Structural modulation of rare earth/noble metal nanocatalysts with enhanced catalytic performances. **Y. Zhang***
- 396.** Low-temperature CO oxidation over Pt/Fe_xO_y catalysts prepared by colloid-deposition method. **M. Jia***, W. Zhang
- 397.** Designing a novel monolithic Ni-SiO₂/SiC foam catalyst for the oxidative methanol dry reforming reaction to produce syngas. **X. Gao**, Q. Wei, G. Yang, Y. Yoneyama, N. Tsubaki*
- 398.** CO₂ hydrogenation over Ni-Cu alloy catalysts supported on Al₂O₃. **R. Sakai**, S. Hosokawa, K. Teramura, T. Tanaka
- 399.** Kinetic model fitting for selective esterification of docosahexaenoic acid. **A. Sharma***, K. Singh, A. Dalai, S.P. Chaurasia

- 400.** Conversion of ethanol to butanol over Ni-based catalysts. **J. Pang**, M. Zheng*, R. Sun, B. Xiao, L. Li, A. Wang, X. Wang, T. Zhang*
- 401.** Sunlight-driven hydrogen peroxide production from water and molecular oxygen by metal-free carbon nitride photocatalysts. **Y. Shiraihi***, Y. Kofuji, T. Hirai

Hyatt Regency Waikiki
Ekahi

Theory and Computation for Efficient Utilization of Energy and Resources (#163)

Organized by: Q. Ge, W. Li, H. Cheng
Presiding: H. Cheng , P. Hu

- 8:00 – 402.** Density functional theory study on electrical double layers. **P. Hu**

- 8:35 – 403.** Transition-metal oxide electrocatalysis. **A. Vojvodic***

- 9:05 – 404.** Aligning energy levels across electrochemical interfaces. **J. Cheng**

- 9:35 – 405.** Molecular modeling in the design of electrically insulating liquids. **N. Davari, P. Åstrand***, M. Unge

9:55 Break

- 10:05 – 406.** Big data analytics: Theoretical concepts, challenges, and hype. **M. Scheffler**

- 10:40 – 407.** New computational method to explore reaction network. **L. Wang**

- 11:10 – 408.** Coarse-grained transport model for the computationally-guided design of next-generation polymer electrolytes. **M.A. Webb**, B.M. Savoie, T.F. Miller

- 11:40 – 409.** First-principle simulations of CO₂ capturing by alcoholamines. **H. Li, M.B. Tsai***

Hawaii Convention Center
Halls I, II, III

Dynamical Processes of Light Harvesting Surfaces (#178)

Organized by: G. Thornton, M. Henderson, H. Onishi, C. Li, G. Herman

Poster Session
10:00 – 12:00

- 410.** Photoexcited carrier dynamics of double-layered PbS/Cds quantum dot sensitized solar cells characterized by transient absorption methods. **K. Sato**, S. Kuwahara, K. Katayama, Q. Shen*

- 411.** Investigation on dye-ion interaction in dye-sensitized solar cells using transient absorption spectra. **R. Hosokawa**, S. Kuwahara, Q. Shen, T. Toyoda, K. Katayama*

- 412.** SrTiO₃ Photocatalysts prepared through solid-state, molten salt, and solvo-thermal method. **Y. Park**, H. Onishi*

- 413.** Time-resolved IR absorption of photo-excited electrons in TiO₂. **T. Mizutani**, H. Onishi*

- 414.** Dynamics of photocarriers in SrTiO₃ studied by transient absorption spectroscopy: Elucidation of the effects of defects. **J.M. Vequizo**, A. Yamakata*

- 415.** Free energy landscape of charge separation in organic disordered materials from first principles simulation. **K. Nishimura***, M. Fujii, K. Yamashita

* Principle Author

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Hyatt Regency Waikiki
Makalo Ballrm

Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188)

Organized by: K. Miyatake, M. Tada, Y. Sung, B. Pivovar, M. Hickner
Presiding: A. Herring, B. Pivovar

8:00 – 416. Development of perfluorinated alkaline membranes and advanced covalently tetherable cations. **B. Pivovar**, M. Sturgeon, H. Long

8:40 – 417. Anion exchange membranes composed of perfluoroalkyl and ammonium-functionalized oligophenylene main chains. **H. Ono***, J. Miyake, K. Miyatake

9:00 – 418. Polymer design of sterically-protected anion exchange membranes. **A.G. Wright**, S. Holdcroft*

9:20 – 419. Stabilization of anion exchange membranes to alkaline conditions for use in fuel cells. **J. Ward**, S. Holdcroft

9:40 Break

9:50 – 420. Next generation polymers for anion exchange membrane fuel cells. **A. Herring***, L. Matthew, D. Knauss, E. Coughlin, G. Voth, T. Witten

10:20 – 421. Structural modification on polystyrene based anion exchange membrane for optimizing membrane properties and performance. **S. Tuli**, R. Elgammal, T. Zawodzinski, T. Fujiwara*

10:40 – 422. Non-platinum catalysts for fuel cells obtained by sacrificial support method. **P. Atanassov***, K. Artyushkova, A. Serov, I. Matanovic, B. Kiefer, B. Halevi

11:10 – 423. Electrocatalysts for H₂/Air(O₂) anion exchange membrane fuel cells: Building a new non-pgm materials set. **A. Serov**, Y. Kim, M. Odgaard, B. Halevi, P. Atanassov

Hyatt Regency Waikiki
Makai Ballrm

Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216)

Organized by: Z. Huang, P. Chen, T. Autrey, Q. Xu, C. Yoon, C. Jensen
Presiding: T. Autrey, C. Buckley

8:00 opening remarks

8:10 – 424. Materials-based hydrogen storage technologies: An overview from the U.S. DOE's perspective. **N.T. Stetson***

8:40 – 425. Heterolysis of molecular hydrogen for energy storage applications. **T. Autrey***

8:55 – 426. High temperature metal hydrides for concentrated solar thermal energy storage. **C. Buckley***, D. Sheppard, T. Humphries, M. Rowles, M. Sofianos, P. Javadian

9:15 – 427. Advances in the formation and regeneration of alane for hydrogen storage. **R. Zidan***, P.A. Ward, J.A. Teprovich , s. greenway, S. Mcwhorter

9:35 – 428. Amino alanes - possible new materials for hydrogen storage. **M. Felderhoff***

9:55 Break

10:05 – 429. Novel H . .H interactions in chemical and metal hydrides. **S. McGrady**

10:25 – 430. Crystal structure analysis of Nb doped Ti-V-Cr hydrogen absorbing alloys using neutron diffraction. **E. Akiba***, S. Itano, H. Hirano, J. Matsuda, K. Ikeda, T. Otomo

10:45 – 431. Enhanced hydrogen generation performance of MgH₂ based hydrides. **L. Ouyang**, M. Zhu

11:05 – 432. Synthesis of metal@carbon hydrides and their enhanced effects on hydrogen storage properties of MgH₂. **Y. Wang**, **Y. Wang**, L. Jiao, H. Yuan

11:25 – 433. Redox reaction kinetics of metal oxides in chemical-looping processes for hydrogen production/storage systems using oxide ion conducting materials. **J. Otomo***, F. Kosaka, Y. Oshima, H. Hatano

11:40 – 434. Synthesis and energy device research of complex hydrides. **S. ORIMO***

Hawaii Convention Center
Halls I, II, III

New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250)

Organized by: Y. Yang, S. Meng, A. Yamada, Y. Sun

Poster Session

10:00 – 12:00

435. Graphene-based nanocomposites anode materials for lithium ion batteries. **H. Kim**, **K. Kim***

436. Toward high-volumetric energy density lithium-ion batteries: Particle density measurements of layered LiCo_{1-x}Ni_xO₂ with 0 ≤ x ≤ 1. **K. Mukai***, H. Nakano

437. Effect of solid phase in fumed silic/lithium electrolyte solution dispersion system. **R. SOGAWA**, S. NAGATA, H. Maki, M. Mizuhata

438. Chemical reaction of organic carbonate on Li anode surface in Li-air battery based on tight-binding quantum chemical molecular dynamics. **K. Watanabe***, Y. Higuchi, N. Ozawa, M. Kubo

439. Exploration of Mn-based oxides micro/nanostructures as anode materials for advanced lithium ion batteries. X. Gu, N. Wang, **J. Yang**, Y. Qian

440. Synthesis and characterization of ordered mesoporous electrode materials for lithium storage. S. Park, P. Kim, H. Lee, G. Park, **J. Kim***

441. Novel lithium ion conducting oxides based on LiSiO₂. **G. Zhao**, I. Muhammed, K. Suzuki, M. Hirayama, R. Kanno*

442. Effects of sulfur electrolyte additives on solid electrolyte interfaces of lithium-ion batteries. **S. Kikuzaki**, C. Yogi, T. Sanada, K. Kojima, M. Katayama, Y. Inada, T. Ohta

443. Li₃V_xMn_{1-x}(PO₄)₃ as a positive electrode material for high rate rechargeable lithium batteries. **J. Park**, S. Myung

444. All solid state batteries using epitaxial-film cathode with a lithium-rich layered rocksalt structure. **M. Hirayama***, Y. Zheng, K. Suzuki, R. Kanno

445. Effects of K-ion doping on electrochemical performance of Na₃V₂(PO₄)₃ cathode materials for Na-ion batteries. **J. Eom***

446. Co-precipitation synthesis of low carbon-coated Li_{0.6}V_{0.4}PO₄ as high-rate cathode materials for lithium ion battery. W. Ma, H. Chen, C. Chang, **Y. Chen-Yang***

447. Synthesis and electrochemical characteristics of nano porous silicon/carbon composite anode for lithium ion battery. **J. Lee***, H. Lee, J. Park

448. Eye-inspired radical scavenger: Polydopamine as an electrolyte additive for improved cycle performance of Li-air batteries. **S. Kim**, J. Choi*, H. Lee*

449. Lithium ion conductor with Argyrodite type structure in the Li-Ge-P-S system. **Y. Inoue**, K. Suzuki, M. Hirayama, R. Kanno

450. Intercalation of sodium and magnesium into boron/carbon materials. **H. Higuchi***, M. Kawaguchi

451. Green, large-scale synthesis of hierarchical nanorod assembly of polyaniline for supercapacitor applications. **D. S***

452. Nickel-manganese oxide on MWCNTs/CFP substrate as supercapacitor electrode. X. Zhang, H. Wang, Y. Huang, **Q. Li***

453. Unique nano-architecture electrodes for high-performance supercapacitor. **G.G. Khan***, A.K. Singh , D. Sarkar

454. Reaction and transport of alkali metal ion on SnO₂ thin film fabricated by liquid phase deposition method. **Y. SHIBATA**, H. Maki, M. Mizuhata

455. Electrocatalytic oxygen evolution by polyanion-based manganese compounds. **T. Takashima***, H. Irie

456. Efficient electrocatalytic electrodes for energy storage devices based on conducting polymers. **P. Talemi***

457. High-energy-density proton redox capacitor using quinonoid compounds couple. **T. Tomai***, D. Komatsu, I. Honma

458. Reversible oxidation of Pt nanoparticles: In situ hard X-ray photoelectron spectroscopy studies under H₂O and MeOH atmospheres. **H. Wang**, Y. Takagi, Y. Uemura, O. Sekizawa, T. Uruga, M. Tada, Y. Iwasawa*, T. Yokoyama*, H. Yoshikawa

459. High contrast and complementary electrochromic device based on a WO₃ film and an organic solution with broadly absorbing from the visible and the infrared. **D. Weng***, M. Li, J. Zheng, C. Xu*

460. Charge/discharge behavior of Co-doped Li₂O of a battery utilizing a redox of oxide and peroxide. **H. Kobayashi***, M. Hibino, Y. Ogasawara, T. Kudo, S. Okuwa, H. Ono, K. Yonehara, Y. Sumida, N. Mizuno

461. Far-red sensitive squaraine dyes with extended II-conjugation toward anchoring group for molecular photovoltaics. G.M. Shivashirpi, N. Fujikawa, G. Kapil, Y. Ogomi, **S.S. PANDEY***, Y. Yamaguchi, S. Hayase

462. Fabrication of graphene/Poly(styrene-sulfonic acid-g-aniline) composites for high performance supercapacitor electrodes. **j. lee**, j. jo, k. Kim, W. Jo*

463. Co₃O₄ supercrystals with enhanced performances in energy storage. **Y. Gong**, S. Lu, H. Chen, C. Wang, **F. Li**

464. Molecular design and photophysical characterization of squaraine dyes with varying fluoroalkyl substituents. **T. Morimoto***, N. Fujikawa, Y. Ogomi, Y. Yamaguchi, S.S. PANDEY, T. Ma, S. Hayase

465. Energy storage by proton-coupled electron transfer reactions of Ru complexes. **D. MOTOYAMA**, H. Ozawa, M. Haga*

466. Investigating small-polarons in Mo/W-BiVO₄: Large implications for solar H₂ production. **V. Jovic***, J. Laverock, A.J. Rettie, J. Zhou, C.B. Mullins, D. Wilson, T. Söhnel, K.E. Smith

467. Porous graphene structure from electrochemical exfoliation for supercapacitor applications. **S. Jung**, H. Jung, J. Kong

468. Performance enhancement of planar heterojunction perovskite solar cells by n-doping of electron transporting layer. **S. Kim**, Bae, W. Jo*

469. Membrane-free wastewater electrolysis cell for decentralized molecular hydrogen production: Current and energy efficiency. **K. Cho***, M. Hoffmann

470. Surface enhanced IR absorption spectro-electrochemistry of immobilized [NiFe] hydrogenase on graphene oxide/Au hybrid electrodes. **H. Gatemala***, L.C. Perez, T. Harris, S. Frielingdorf, O. Lenz, C. Thammacharoen, S. Ekgasit, I.M. Weidinger, A. Fischer, N. Heidary*, K.H. Ly*, I. Zebger*

471. Creation of chiral ionic plastic crystals and its proton conductivity. **T. Yamada***, M. Matsuki, N. Kimizuka

472. Interrelation between processing condition, morphology, crystal orientation, and efficiency of CH₃NH₃PbI₃-based perovskite solar cells. **S. Bae**, S. Han, T. Shin, W. Jo*

Hyatt Regency Waikiki
Kou Ballrm

Artificial Photosynthesis: Bio-inspired Chemistry for Solar Fuel Production (#278)

Organized by: H. Hashimoto, Y. Amao, J. Zhang, T. Moore, B. Koivisto

Presiding: Y. Amao, H. Hashimoto, B.D. Koivisto, T.A. Moore, J. Zhang

8:00 – 473. Mechanism of light-induced water splitting – learning from nature's ingenious concept. **W. Lubitz***

8:30 – 474. Molecular photosynthesis: Such stuff as dreams are made on. **M. Bonchio***

8:45 – 475. In-situ passivation layer protected Si photoanode with sparse catalysts for stable and quantitative solar water oxidation. **K. Sun**, W.G. Hale, B.S. Brunschwig, N.S. Lewis

9:00 – 476. Birnessite as structural motif for the development of oxygen evolution reaction (OER) electrocatalysts. **J.H. Baricuatro***, F.H. Saadi, A. Carim, J.M. Velázquez, M.P. Sorriaga

9:15 – 477. Bio-inspired catalytic systems and technological applications of hydrogen. **V. Artoro***

9:45 – 478. Proton-coupled electron transfer processes in artificial photosynthesis. **L. Hammarström***, S. Glover, G. Parada, T. Marke, M. Bourrez, p. Dongare, S. Ott

10:00 – 479. Evaluation of oxidation ability for plasmon-induced charge separation: Approach from coordinative dissolution and surface passivation of gold nanoparticles. **H. Nishi***, T. Tatsuma*

10:15 – 480. Bio-nano photocatalytic systems for solar hydrogen production. **E. Rozhkov***, P. Wang

10:30 – 481. Photocatalytic hydrogen production using carbon nitrides with enzymatic and synthetic biomimetic co-catalysts. **C.A. Caputo**, M.A. Gross, E. Reisner

10:45 – 482. Novel metal-peptide conjugates for CO₂ reduction catalysts. **H. Ishida***

11:15 – 483. BODIPY as a non-innocent π-spacer in organic dye motifs: Toward next-generation photovoltaic applications. **B.D. Koivisto***

11:30 – 484. Achieving enzyme-like behavior with amino acids and peptides in the outer coordination sphere of hydrogenase mimics. **W. Shaw***, A. Dutta, J. Roberts, A. Jain, M. Reback

11:45 – 485. Artificial light-driven proton pumps as mimics for natural photosynthesis. **C.D. Sanborn**, R. Reiter, W. White, **S. Ardo**

Hyatt Regency Waikiki
Mauka Ballrm

Homogeneous Catalysis Methodologies for the Upgrading of Biomass Derived Molecules (#301)

Organized by: J. Gordon, R. Baker, T. Ikariya

Presiding: T. Ikariya

8:00 – 486. Strategies for biofeedstock processing via tandem catalytic C-O hydrogenolysis. **T.J. Marks**

8:35 – 487. Catalytic conversion of renewable resources into bulk and fine chemicals. **J.G. de Vries***

9:10 break

9:20 – 488. Commercialization of olefin metathesis for use in the world's first biorefinery plants. **R.L. Pederson***

9:45 – 489. Hydrogenation and dehydrogenation processes based on bifunctional Ru and Ir complexes bearing protic amine chelate ligands. **Y. Kayaki***

10:10 – 490. Hydrogen management for transformation of CO₂- and biomass-derived feedstock using molecular surface. **S. SAITO***

10:35 break

10:45 – 491. High efficient tetradentate ruthenium catalyst for esters reduction. **X. Zhang**

* Principle Author

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11:10 – 492. Bifunctional Ir/NH hydrogenation catalyst with a reversed NH/NMe substitution effect. **P.A. Dub***, B.L. Scott, J. Gordon*

11:35 – 493. Green synthesis of paracetamol from renewable limonene. **M. Hutchby***, W. Cunningham, S.D. Bull

Hyatt Regency Waikiki
Elima

Challenges in Second Generation Biofuels: Processing, Stability, and Usage (#378)

Organized by: J. Fu, J. Chen, S. Turn, Z. Tao
Presiding: J. Fu, S.Q. Turn

8:00 Opening Remarks

8:05 – 494. Catalytic biomass pyrolysis and bio-crude upgrading for advanced biofuels production. **D.C. Dayton***, O. mante, J. Peters, D. Barbee, K. Wang, R. Gupta

8:40 – 495. Biomass oxidation: Formyl C–H bond activation by the surface lattice oxygen of regenerative CuO nanoleaves. **Y. Yang**

9:15 – 496. Biofuel synthesis in supercritical fluids. **J. Kim***

9:50 Break

10:05 – 497. Continuous enzymatic hydrolysis of biomass in a membrane reactor. **R. Wickramasinghe***, M. Malmali, J. Sticke

10:40 – 498. Role of ultrasound in the renewable energy production and utilization: Comparison with Co-solvent and micro-wave. **Y. Maeda***, H.T. Truong, K. Noro, N. Takenaka, L.V. Boi

11:15 – 499. Comparative proteome analysis for biodiesel metabolism using a novel *Moniliella wahieum* Y12 isolate. **D. Si***, T. Ching, D. Roettger, B. Yoza, S. Masutani, Q.X. Li

Thursday Afternoon

Hyatt Regency Waikiki
Ekahi

Theory and Computation for Efficient Utilization of Energy and Resources (#163)

Organized by: Q. Ge, W. Li, H. Cheng
Presiding: H. Cheng , J. Li

13:00 – 500. On the role of hydroperoxy (·OOH) radical in oxidation reactions at bulk gold surfaces. **J. Li***, C. Chang, X. Yang

13:35 – 501. First-principles perspective on TiO₂ surface photocatalysis. **J. Zhao***

14:05 – 502. Catalyst design for improving kinetics of oxygen evolution reactions in Li-O₂ battery. **J. Liu***

14:35 – 503. Li₂ZrO₃: A potential cathode material for lithium ion batteries. **S. Huang**, B. Wang, B. Wilson, Y. Fang, A. Stein, D.G. Truhlar

14:55 Break

15:05 – 504. Strong hydrogen bond can enhance and inhibit water/methanol dissociation on TiO₂ surface. **H. Fan**

15:35 – 505. Molecular design rules of D-A nanofibril interface for high photoconductivity and photovoltaic performance. **X. Yang***

16:05 – 506. Theoretical study on electronic processes at the donor/acceptor interface in organic solar cells. **Y. Yi***, X. Shen, G. Han

16:35 – 507. Chemical solutions for the hysteretic effects in mixed organic-inorganic perovskites: A theoretical analysis. **G. Giorgi***, K. Yamashita

Hyatt Regency Waikiki
Maloko Ballrm

Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188)

Organized by: K. Miyatake, M. Tada, Y. Sung, B. Pivovar, M. Hickner
Presiding: Y. Sung, S. Yoo

13:00 – 508. Nanoarchitecture and catalyst designs for fuel cell application. **S. Yoo**, N. Jung, D. Chung, J. Ryu, H. Park, J. Jang, H. Kim, Y. Sung

13:40 – 509. Highly active and durable extended surface electrocatalysts. **S.M. Alia***, K. Neyerlin, S. Pylypenko, S. Kocha, B. Pivovar

14:00 – 510. Mechanism of redox processes of Pt-M (M = Co, Ni) PEFC cathode electrocatalysts for voltage cycling studied by *in situ* time-resolved XAFS. **N. Ishiguro***, S. Kitayakarn, O. Sekizawa, T. Uruga, K. Nagasawa, T. Yokoyama, M. Tada

14:20 – 511. Nanoparticle designs with high activity and durability as electrocatalyst for fuel cells. **D. Chung, H. Kwon, Y. Sung***

15:00 Break

15:10 – 512. Strategies for design and synthesis of highly efficient non-precious metal catalysts using metal-organic frameworks and porous organic polymers. **D. Liu***

15:40 – 513. Strategy to improve efficiency of graphene-based ORR electrode for PEMFC. **S. Woo***, M. Chung

16:00 – 514. Highly active nanostructured carbon-based non-precious metal electrocatalysts for the oxygen reduction reaction. **S. Joo***

16:20 – 515. Effects of major air contaminants on the performance of fuel cells with nonplatinum group metal cathode catalysts. **T.V. Reshetenko***, A. Serov, S. Starika, I. Matanovic, K. Artyushkova, J. St-Pierre, P. Atanassov

Hyatt Regency Waikiki
Makai Ballrm

Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216)

Organized by: Z. Huang, P. Chen, T. Autrey, Q. Xu, C. Yoon, C. Jensen
Presiding: P. Chen, C.M. Jensen

13:00 – 516. Ammonia - the ideal chemical storage material? **B. David***, M.O. Jones, J.W. Makepeace, T.J. Wood, h. hunter

13:30 – 517. Ammonia as a hydrogen storage material. **Y. Kojima**

13:50 – 518. Accelerated DFT-based design of materials for ammonia storage. **T. Vegge***

14:10 – 519. Amides, amines, and ammonia as hydrogen carriers. **P. Chen***, J. Guo, P. Wang, F. Chang, P. Yu, G. Wu

14:25 – 520. Hydrogen release from irradiated ammonia-borane: A computational study. **M. Gutowski***, D. Bellshaw, R. Hernandez

14:40 – 521. Syntheses of amine boranes as potential hydrogen storage materials. **X. Chen***, Y. Guo, H. Li

15:00 break

15:10 – 522. Hydrogen storage properties of nanosized MgH₂-0.1TH₂ prepared by ultrahigh-energy-high-pressure milling. **J. Lu, Z.Z. Fang**

15:30 – 523. Development of boron hydrides. **D.M. Schubert**

15:50 – 524. A chemist's walk through a solid chemical hydrogen fuel cartridge. **A.M. Fisher**

16:10 – 525. Solid state hydrogen storage materials: Key issues. **X. Yao**

16:30 – 526. Mechanistic studies of the reversible hydrogenation of boranes to borohydrides under moderate conditions. **C.M. Jensen***, T. Autrey, S. ORIMO, M. Chong, J. Wang, M. Matsuo

16:45 – 527. Understanding and controlling the hydrogen release and uptake in complex metal hydrides. **V. Stavila***, E. Majzoub, J. Vajo, B. Wood, L. Klebanoff

Hyatt Regency Waikiki
Kou Ballrm

New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250)

Organized by: Y. Yang, S. Meng, A. Yamada, Y. Sun

13:00 – 528. Sodium insertion materials for designing 4-volt class battery. **S. Komaba***, K. Kubota, M. Dahbi

13:25 – 529. Selected metal disulfides for fast and stable Na⁺ intercalation/de-intercalation. **J. Chen***, Y. Liu*, X. Liu, L. Jiao

13:50 – 530. High performance iron based cathode material for sodium-ion batteries. **K. Chung**, G. Ali, S. Oh, S. Kim, J. Kim, B. Cho

14:10 – 531. Ordered and disordered O₃-Na₂RuO₃ as high performance positive electrode materials for Na-ion batteries. **B. Mortemard du Boisse***, G. Liu, J. Ma, N. Shin-ichi, H. Kiuchi, Y. Harada, J. Kikkawa, Y. Kobayashi, M. Okubo, A. Yamada

14:25 – 532. Solid state ²³Na NMR study on reaction mechanism of MXene Ti₃C₂T_x in non-aqueous Na⁺ electrolyte. **S. Kajiyama**, H. Iinuma, R. Morita, K. Gotoh, M. Okubo, A. Yamada

14:40 – 533. All-solid-state Li-ion microbatteries based on vertical arrays of titania nanotubes. **T. Djenizian**

14:55 Break

15:05 – 534. Na-air batteries: Understanding of mechanisms and rechargeability. **X.A. Sun***

15:30 – 535. Cathode reactions and basic property of lithium peroxide batteries. **M. Hibino***, H. Kobayashi, K. Harada, Y. Ogasawara, N. Mizuno

15:55 – 536. Safety-reinforced, wide voltage window and ambient temperature polymer-based solid polymer electrolyte for high-performance lithium batteries. **J. Zhang, J. Zhao, L. Yue, Z. Liu, G. Cui**

16:10 – 537. Mo₂C-CNT cathode for lithium-oxygen battery. **W. Kwak**, K. Lau, K. Amine, L. Curtiss, Y. Sun*

16:25 – 538. Building better lithium-sulfur batteries. **N. Ding**, Z. Liu, Y. Zong

Hyatt Regency Waikiki
Mauka Ballrm

Homogeneous Catalysis Methodologies for the Upgrading of Biomass Derived Molecules (#301)

Organized by: J. Gordon, R. Baker, T. Ikarya
Presiding: R. Baker

13:00 – 539. Microbial synthesis of glucaric acid: A case study for the design, assembly, and improvement of a biosynthetic pathway for value-added products. **K.L. Prather**

13:35 – 540. Metabolic engineering of bacteria for production of oleochemicals. **B.F. Pfleger***

14:10 break

14:20 – 541. Regulation of the endogenous xylose utilization pathway by the lysine acetyltransferase NuA4 in *Saccharomyces cerevisiae*. **K. Baetz***

14:45 – 542. Real-time imaging of biomass deconstruction using small-angle neutron scattering. **H. O'Neill**, S. Pingali, P. Loukas, V. Urban, B. Evans, P. Langan, J. Smith, Y. Nishiyama, B. Davison

15:10 break

15:20 – 543. Improving cellulase activity for biomass conversion. **S.R. Decker**, L. Taylor II, J.L. Linger, T.A. Vander Wall, J.O. Baker, V. Subramanian, G.T. Beckham, M.E. Himmel

15:45 – 544. Biocatalytic route to commodity chemicals: Creation of a thermostable dehydroshikimate dehydratase. **D.T. Fox***, L. Harrington, G. Canales, K. Hotta, R. Del Sesto, M.T. Janicke, C. Strauss, T. Kern, A. Koppisch*, R. Jha*

16:10 – 545. One-pot synthesis of levulinic acid from cellulose in SO₃H-functionalized ionic liquids. **B. Wang***

Hyatt Regency Waikiki
Elima

Challenges in Second Generation Biofuels: Processing, Stability, and Usage (#378)

Organized by: J. Fu, J. Chen, S. Turn, Z. Tao
Presiding: J. Fu, S.Q. Turn

13:00 Opening Remark

13:05 – 546. Advancements of pennycress as a biofuel and the synthesis of estolides thereof. **S.C. Cermak***, T.A. Isbell, R.L. Evangelista, B. Moser, R.E. Murray

13:40 – 547. High pressure reactors for the conversion of FFAs and lipids to biofuels. **J.A. Hestekin***

14:15 – 548. Practice of the conceptual one-pot processing of pretreatment, saccharification, and ethanol fermentation of lignocellulose. **K. Kim***

14:50 Break

15:05 – 549. Assessment of the fast pyrolysis behaviour of tropical biomass species as a function of volatile residence time and temperature. **T.J. Morgan***, S.Q. Turn

15:40 – 550. Measurement of NO_x in biodiesel exhausts by surface modified air-dragged aqua-membrane-type denuder (MADAM) sampling and fluorescence detector. **H.T. Trinh***, N. Takemura

16:15 – 551. Effects of aromatic type and concentration on hydroprocessed renewable diesel characteristics. **J. Fu**, S.Q. Turn

Thursday Evening

Hyatt Regency Waikiki
Kou Ballrm

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli
Presiding: N.C. Anderson, A. Dalai

19:00 Opening Remarks-Nanocatalysis-Structural Study-II

19:02 – 552. Black silicon: Nanostructuring to improve catalyst/semiconductor interfaces for photochemical water splitting. **N.C. Anderson***, N. Neale, J.A. Aguilar

19:22 – 553. Tuning nanocrystals for oxygen reduction. **S. Guo**

19:42 – 554. Zeolites with nanometer diffusion lengths: Mechanistic implications in shape selective catalytic conversion of methanol-to-hydrocarbons. **D.M. Miller**, R. Khare, A. Bahn*

20:02 – 555. Mo_MmetalO_x as a case study in engineering industrially important heterogeneous catalysts at the nanoscale level. **J.W. Kauffman***

20:22 – 556. Double perovskite structure GaBaCo_{2-x}Fe_xO_{5+δ} nanoparticles synthesised by a biomimetic approach: Estimates of diffusivity and electrochemical performance. **M. Haider***, U. Anjum, M. Sardar, N. Khatton, N. Sinha

* Principle Author

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Hawaii Convention Center
Halls I, II, III

Theory and Computation for Efficient Utilization of Energy and Resources (#163)

Organized by: Q. Ge, W. Li, H. Cheng
Poster Session
19:00 – 21:00

557. Multiscale simulation for lithium-ion battery focused on SEI film growth and capacity fade. **C. Shinagawa***, H. Ushiyama, K. Yamashita
558. Density functional theory study on the catalytic activation of carbon dioxide on transition metal surfaces. J. Ko, B. Kim, J. Han

559. Screening of ORC working fluids for waste heat recovery in automotive and marine engineering by COSMOTHERM and DetailSimORC. **A. Klamt**, J. Schwöbel, M. Preißinger

560. Comparative computational study of acetic acid adsorption on three crystalline (anatase, rutile, B) and amorphous surfaces of TiO₂. **S. Manzhos***, G. Giorgi, K. Yamashita
561. Computational studies of electrolyte oxidation to develop high-voltage electrolytes. **D. Kim**, H. Park, J. Seo, I. Park, Y. Kang, J. Park, S. Doo

562. Barrier free conversion of NO gas to ammonia over iron oxide clusters. **K. Takahashi***

563. Theoretical studies on the intercalation mechanism of Li/Na ions in Ti₂C: Anode material for Li/Na ion battery. **S. Kurahashi***, H. Ushiyama, K. Yamashita

564. Ab initio study on the initial steps of the pyrolysis and oxidation of aviation fuels and analogs. **A. Jamal***, K. Morokuma

Hyatt Regency Waikiki
Maloko Ballrm

Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188)

Organized by: K. Miyatake, M. Tada, Y. Sung, B. Pivovar, M. Hickner
Presiding: K. Miyatake

19:00 – 565. Low temperature biomass-to-electricity direct fuel cell. **Y. Deng**
19:20 – 566. High efficient biomass-to-hydrogen conversion by polyoxometalate solution catalyzed electrolysis. **Y. Deng***

Hawaii Convention Center
Halls I, II, III

Challenges in Second Generation Biofuels: Processing, Stability, and Usage (#378)

Organized by: J. Fu, J. Chen, S. Turn, Z. Tao
Presiding: J. Fu, S.Q. Turn

Poster Session
19:00 – 21:00

567. Biomass to biofuels: Elements of the Hawaii Natural Energy Institute's alternative fuels research. **S.Q. Turn***, H. Cui, J. Fu, D. Harris, D. Li, T.J. Morgan, A. Mousavi, T. Petrik, W. Plavis, S. Taniguchi, B. Zezulova
568. Advanced bioethanol production with acetic acid fermentation from lignocellulosics. **S. Sakai***, H.F. Rabemananjara, E. Minami, H. Kawamoto

569. Advanced bioethanol production with acetic acid fermentation from lignocellulosics:(1) Hot-compressed water treatment of lignocellulosics to decomposed products. **E. Minami***, Y. Osada, S. Saka
570. Advanced bioethanol production with acetic acid fermentation from lignocellulosics:(2) Acetic acid fermentation of decomposed products to acetic acid. **H.F. Rabemananjara***, K. Yoshimizu, P. Jusakulvijit, S. Saka

571. Advanced ethanol production with acetic acid fermentation from lignocellulosics: (3) Hydrogenolysis of acetic acid to ethanol. **H. Kawamoto**, Y. Ito, T. Fujii, S. Saka*

572. Corrosion of 1018 carbon steel in static seawater/diesel (petrol and renewable) mixtures. **J.A. Kealoha***, S. Li, S.P. Donachie, L.H. Hihara

573. Biogas production from the wastewater including acetonitrile. **M. Onodera***, T. Terui, T. Satoh, S. Watanabe, M. Imai, K. Satoh, S. Takesono

574. Renewable diesel production from plant oils by hydrothermal hydrogenation and decarboxylation. **Y. Sugami***, E. Minami, S. Saka

575. Thermo-alkaline lipase from a new thermophile *Geobacillus thermodenitrificans* AV-5 with potential application in biodiesel production. **L. Christopher***, V. Zambrano, H. Kumar, L. Malek

576. Advanced bioethanol production from nipa sap via acetic acid fermentation. **D.V. Nguyen***, H.F. Rabemananjara, S. Saka

577. Effects of supercritical hexane on the catalytic deoxygenation of oleic acid: Kinetic perspective. **M. Park***, Y. Woo, J. Park, J. Choi, J. Ha, D. Suh

578. Improving oxidation stability of biodiesel by antioxidant derived from spent coffee ground. **M. Todaka**, W. Kowahakul, H. Masamoto, M. Shigematsu*

Friday Morning

Hyatt Regency Waikiki
Ekahi

Theory and Computation for Efficient Utilization of Energy and Resources (#163)

Organized by: Q. Ge, W. Li, H. Cheng
Presiding: Q. Ge, D. Mei

8:00 – 579. Mechanistic insights into selective conversion of biomass-derived intermediates over supported metal catalysts in aqueous media. **M. Neurock***

8:30 – 580. Fundamental insights into aqueous-phase dehydration of cyclohexanol in H-BEA zeolite. **D. Mei**, J.A. Lercher

9:05 – 581. Biomass oxidation: Formyl C–H bond activation by the surface lattice oxygen of regenerative CuO nanoplates. **Y. Yang**

9:35 – 582. Density functional theory study of hydrodeoxygénération of phenolics over Ru/TiO₂. B. Baek, **L.C. Grabow***

9:55 Break

10:05 – 583. Computational studies of catalytic materials for Li-air batteries. **L.A. Curtiss***, k. Lau, L. Cheng, u. das, C. Liu

10:40 – 584. Computational studies of materials interfaces for optimization of energy storage and conversion devices. **V. Lordi***

11:10 – 585. Understanding electric energy storage by supercapacitors. **D. Jiang***

11:40 – 586. Multiscale simulation based on first-principles and reactive force field for Li-ion batteries. **S. Han***, H. Jung, B. Yeo, K. Yun, M. Lee, K. Lee

Hyatt Regency Waikiki
Maloko Ballrm

Current Status and Future Prospect of Polymer Electrolyte Fuel Cells (#188)

Organized by: J. Fu, J. Chen, S. Turn, Z. Tao
Presiding: J. Fu, S.Q. Turn

8:00 – 587. Reaction distributions inside running PEFCs analyzed by novel experimental techniques and numerical simulations. **J. Inukai***, Y. Nagumo, M. Yoneda, H. Nishide, M. Watanabe

8:40 – 588. In situ XAFS, STEM, and electrochemical studies on degradation processes of Pt-based PEFC cathode catalysts by repeated feed-gas exchange procedures. **G. Samjeské**, K. Higashi, S. Takao, O. Sekizawa, T. Kaneko, S. Nagamatsu, K. Nagasawa, T. Uruga, Y. Iwasawa*

9:00 – 589. 3D imaging of the distribution and local structure of Pt electrolycatalyst in PEFC MEA by in situ CT-XAFS. **H. Matsui***, O. Sekizawa, N. Ishiguro, T. Uruga, T. Yokoyama, M. Tada

9:20 – 590. Investigation of PEFC cathode degradation mechanism through in-situ SEM/STEM techniques. **A. Hayashi***, M. Kitamura, Z. Noda, K. Sasaki

9:40 Break

9:50 – 591. Characterizing polymer electrolyte fuel cell materials by soft X-ray scanning transmission X-ray microscopy. **A.P. Hitchcock***, N. Appathurai, V. Berejnov, D. Susac, J. Stumper

10:20 – 592. 3D microstructure of PEFC electrodes: Activity and durability. **K. Artyushkova***, M. Workman, B. Halevi, A. Serov, P. Atanassov

10:40 – 593. Oxygen mass transport at the Pt/ionomer interface: The effect of relative humidity. **D. Novitski***, S. Holdcroft

11:00 – 594. Large scale molecular dynamics simulation of the transport phenomena of materials in polymer electrolyte fuel cell. **T. Tokumasu***

11:30 Closing remark

Hyatt Regency Waikiki
Makai Ballrm

Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216)

Organized by: Z. Huang, P. Chen, T. Autrey, Q. Xu, C. Yoon, C. Jensen
Presiding: Z. Huang, Q. Xu

8:00 – 595. Carbon dioxide - formic acid cycle for hydrogen/energy storage and delivery. **G. Laurenczy***

8:30 – 596. CO₂-facilitated hydrogen release from ammonia borane complex. **J.W. Lee***

8:50 – 597. CO₂ mediated chemical hydrogen storage for fuel cell technology. **C. Yoon**, S. Nam

9:10 – 598. Hydrogen production by dehydrogenation of formic acid using homogeneous iridium catalysts. **Y. Himeda***, H. Kawanami, J.T. Muckerman, E. Fujita

9:30 – 599. Continuous high-pressure hydrogen evolution system with formic acid without compressing. **H. Kawamani***, M. Iguchi, Y. Manaka, Y. Himeda

9:50 – 600. Metal nanoparticle-catalyzed hydrogen generation from liquid-phase chemical hydrides. **Q. Xu**

10:10 break

10:20 – 601. Mechanistic investigation of metal dodecaborates for energy storage. **H. Li***, L. He, E. Akiba

10:40 – 602. Developing new complex hydrides for hydrogen storage and related structural studies. **H. Wu***

11:00 – 603. Structural and dynamical trends in alkali-metal silanides characterized by neutron scattering methods.

T.J. Udovic*, W. Tang, J. Chotard, W. Zhou, R. Janot, J.J. Rush, A.V. Skripov

11:20 – 604. High throughput inelastic neutron scattering, from fiction to reality. **A.J. Ramirez-Cuesta**, Y. Cheng, L. Daemen

11:40 – 605. Hydrogen storage materials composed of lithium hydride and conjugated macromolecules. **A. Yoshida***, Y. Mori, S. Naito, W. Ueda

Hyatt Regency Waikiki
Kou Ballrm

New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250)

Organized by: Y. Yang, S. Meng, A. Yamada, Y. Sun

8:00 – 606. Expanding electrochemical stability window of electrolytes to enable more powerful battery chemistries. **K. Xu***

8:25 – 607. Insight into electrochemical stability of battery electrolytes and transport properties of SEI model compounds from modeling. **O. Borodin**, M. Olguin, C. Spear, K. Leiter, D. Bedrov, J. Knap

8:40 – 608. Investigating 3D structure of the surface film on silicon/lithium metal anode for lithium batteries by scanning force curve method. **J. Zheng***, W. Li, G. Chu, H. Li

8:55 – 609. 4V operating voltage, flexible quasi solid state electrolyte with EMITFSI/cross-linked PV/aramid composite for supercapacitor. **J. Yoo**, H. Kim, D. You, B. Kim, Y. Ahn, S. Cho, Z. Yin, Y. Kim*

9:10 – 610. Soft X-ray spectroscopy of surfaces and interphases in batteries: Problems and potentials. **W. Yang***

9:35 – 611. Neutron scattering studies of large polyhedral hydro-closoborates of sodium and lithium: Implications of structure and anion reorientational mobility on superionic conduction. **T.J. Udovic***, W. Tang, V. Stavila, N. Verdal, H. Wu, W. Zhou, J.J. Rush, A.V. Skripov

9:50 Break

10:00 – 612. All-solid-state and aqueous Li-ion batteries. **C. Wang***

10:25 – 613. Layered transition metal silicates as sustainable materials for electrochemical energy storage. **S. Zhou**, B. Lopez-Bermudez, **B.C. Melot**

10:40 – 614. Rational design and synthesis of new battery materials via in-situ studies. **F. Wang***

11:05 – 615. In situ neutron depth profiling for revealing Li-ion battery processes using neutrons. **A. Co***

11:20 – 616. Investigation of discharge products in the Li-S battery using in-situ ⁷Li NMR coupled with ab initio structure search calculations. **K. See**, M. Leskes, J.M. Griffin, S. Britto, P.D. Matthews, A. Emly, A. Van der Ven, D.S. Wright, A.J. Morris, C.P. Grey, R. Seshadri

11:35 – 617. Degradation mechanism of LiNi_xCo_yMn_zO₂ cathodes at high charge-cut-off-voltages in lithium ion batteries. **J. Zheng***, J. xiao, P. Yan, Q. Li, C. Wang, J. Zhang*

Hyatt Regency Waikiki
Elma

Advances in Microwave Green Chemistry (#360)

Organized by: T. Matsumura, S. Yanagida, R. Varma, K. Jin, S. [ohuchi@bio.kyutech.ac.jp]

Presiding: G.B. Dudley, H. Koshiba, R.S. Varma, S. Yanagida

8:00 opening Remark

8:05 – 618. Sustainable routes to organics and nanomaterials via microwave-assisted reactions. **R.S. Varma**

8:35 – 619. Microwave effect on enantioselective catalysis. **T. Yamada**

8:55 – 620. Existence of and mechanism for microwave-specific rate enhancement of organic reactions in homogeneous solution. **A.E. Stiegman**, G.B. Dudley

9:15 – 621. Microwave effect on Fischer esterification. **H. Koshiba***

9:35 – 622. High-throughput acquisition of reaction progress in a microwave reactor. **D. Yu***, A.F. Jones, C.A. Posadas, G.B. Dudley, J. Hein

9:55 – 623. Selective microwave heating of homogeneous solutions. **G.B. Dudley***

10:15 Break

* Principle Author

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onlineprogram

10:30 – 624. Microwave thermal effects and molecular modeling. **S. Yanagida***, T. Matsumura
11:00 – 625. Classification and estimation methods of organic reactions under microwave condition. K. Uchihiro, N. Iwahashi, **S. Ohuchi***
11:20 – 626. Development of microwave synthesis of platinum metal complexes. **T. Matsumura***, **Y. Masuda**, **S. Yanagida**, T. Watanabe, T. Mitani
11:40 poster review

Hyatt Regency Waikiki
Mauka Blrnm

Global Strategies for Algal Biomass for Bioenergy and Biorefinery (#407)

Organized by: A. Kondo, J. Yang,
Y. Yoshikuni
Presiding: A. Kondo

8:00 Opening remark
8:05 – 627. Some recent approaches to produce bioenergy using cyanobacteria in Japan. **M. Ohmori***
8:45 – 628. Creation of heat and acid tolerant algae toward high biomass production. **S. Miyagishima***
9:05 – 629. Enhanced lipid production in the oleaginous diatom *Fistulifera solaris* by metabolic engineering. **T. Tanaka***, K. Osada, C. Takahashi, M. Muto, Y. Maeda, T. Yoshino
9:25 – 630. Potential of piggy wastewater for mixotrophical cultivation of *S. quadrivittata*. **W. Choi**, H. Kim, A. Chae, H. Seo, J. Park, K. Song*

9:45 Break

10:00 – 631. Laminarin hydrolysis by glycoside hydrolase family 55. T.E. Takasuka, C.M. Bianchetti, K. Deng, E.T. Beebe, L.F. Bergeman, S. Singh, S. Deutsch, P. Adams, B. Simmons*, T.R. Northen*, **B.G. Fox***
10:20 – 632. In situ transesterification of wet microalgae under homogeneous acid catalysts. **J.W. Lee**
10:40 – 633. Development of novel sensor functioning in *Synechocystis* cells using *Arabidopsis* ethylene sensor. M. Kawaguchi, Y. SHIRAIWA, I. Suzuki*
11:00 – 634. Inhibiting growth of contaminated phytophagous protists in algal cultures by controlling the phototoxicity of chlorophylls. **Y. Kashiyama***, J. Kawahara, M. Nakazawa, T. Ishikawa, T. Tanaka, T. Yoshino, H. Tamiaki

Friday Afternoon

Hyatt Regency Waikiki
Ekahi

Nanostructured Oxides for Energy Harvesting and Water Splitting (#171)

Organized by: F. Rosei, Z. Wang, E. Diau, A. Vomiero, X. Sun
13:00 – 635. Morphology control and stability of methylammonium lead iodide solar cells. **U. Bach**
13:30 – 636. Semiconducting quantum dots and metallic nanoparticles sensitized ZnO and Si nanowires-array photoelectrodes for water splitting. **R. Liu**, S. Hu
14:00 – 637. General formation of complex tubular nanostructures of metal oxides and their applications energy storage and conversion. **G. Zhang**
14:15 – 638. Engineering complex, layered metal oxides: High performance nickelate nanostructures for oxygen exchange and reduction. **E. Nikolla**
14:30 coffee break
15:00 – 639. Electrodes for photoelectrochemical cells: Design of semiconductor nano-architectures for structure-driven functional performances. **I. Concina***, R. Milan, G.S. Selopal, G. Sberveglieri
15:30 – 640. Metallic nanoparticles-doped peptide systems: Morphological and luminescent properties. **T.D. Martins**, D.L. Dias, A.C. Ribeiro, H.S. Camargo
16:00 – 641. Solution processed organic/inorganic photovoltaics. **C. Luscombe***

16:30 – 642. Nanoscale (111) faceted rock-salt metal oxides. **R.M. Richards**, G. Leong, C. Cadigan, F. Lin
16:45 – 643. Noble metals containing polyoxoniobates. **P.A. Abramov**, M.N. Sokolov

Hyatt Regency Waikiki
Makai Blrnm

Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216)

Organized by: Z. Huang, P. Chen, T. Autrey, Q. Xu, C. Yoon, C. Jensen
Presiding: B. David, N.T. Stetson

13:00 – 644. Hydrogen storage in nanomaterials. **H. Kitagawa***
13:30 – 645. Novel platinum-based catalyst for methylcyclohexane dehydrogenation in hydrogen storage and utilization technology. **Y. Hisamatsu**, K. Yamamoto, K. Tanaka, Y. Bandai, Y. Kohno, R. Watanabe, C. Fukuhara
13:45 – 646. Recent progress in hydrogen storage on MOFs. **M. Hirscher***
14:05 – 647. Metal-organic framework based materials for clean hydrogen energy utilization. **R. Zou***

14:25 – 648. Advances in hydrogen sorption: Sorbent and hybrid sorbent-hydride, characterization, and validation. P.A. Parilla, k.E. hurst, M. Olsen, J. blackburn, **T. Gennett***
14:45 – 649. Molecular hydrogen storage in filled ice structures. **L. Hakim***, S. Ulfa, M. Matsumoto, K. Koga, H. Tanaka

15:00 break
15:05 – 650. Clusters and hydrogen storage: Convergence of two parallel fields. **P. Jena***
15:25 – 651. Clathrate hydrates as materials for hydrogen storage applications: Theoretical aspects. **R. Belosludov***
15:45 – 652. Bis-BN cyclohexane: A remarkably kinetically stable chemical hydrogen storage material. **S. Liu***

16:05 – 653. Synthesis of new B₃H₈ compounds for hydrogen storage. **Z. Huang**
16:20 – 654. Hydrazine borane N₂H₄BH₃ and alkali hydrazinodiborane derivatives MN₂H₄BH₃ (M = Li, Na and K) as chemical hydrogen storage materials. **U.B. DEMIRCI**

Hyatt Regency Waikiki
Kou Ballrm

New Generation of Electrochemical Energy Storage and Conversion System: Materials, Interface and In-situ Techniques (#250)

Organized by: Y. Yang, S. Meng, A. Yamada, Y. Sun

13:00 – 655. Engendering anion resistance and its implication in electrocatalysis of energy conversion, storage, and efficiency. **S. Mukerjee***, K. Strickland, U. Tylus
13:25 – 656. Does it have to be carbon? Metal anodes in microbial fuel cells and related bioelectrochemical systems. **I. Schmidt**, A. Baudler, M. Langner, A. Greiner, U. Schröder*

13:40 – 657. Development of functional nanographenes toward next generation fuel cells and lithium ion batteries. **H. Wang***, H. Yen, G. Wu, M. Zhou
13:55 – 658. Transition-metal oxides efficient bifunctional catalysts for high performance rechargeable zinc-air batteries. **Z. Liu***

14:10 – 659. Bioinspired electroactive organic molecules for aqueous redox flow batteries. **J. Schrier***

14:25 – 660. Enhancing grain boundary ionic conductivity in ceramic composites for energy conversion and storage. Y. Lin, S. Fang, D. Su, **K.S. Brinkman**, F. Chen

14:40 Break
14:50 – 661. Interaction of polysulfide with nano-structured metal oxides. **V. Murugesan***, A. Dissanayake, C. Szymanski, M. Nandasiri, p. Bhattacharya

15:05 – 662. Structure and chemical state of electrochemically Li inserted Si(111) studied by scanning electron microscopy and soft X-ray emission spectroscopy. **N. Aoki**, T. Kondo*, K. Uosaki*

15:20 – 663. New conversion-type cathode, nano-sized copper phosphate for rechargeable Li batteries. **Y. Yang**, G. Zhong, J. Bai, P. Duchesne, M. Matt, Q. Li, X. Hou, J. Tang, Y. Wang, Z. Gong, P. Zhang, R. Fu

15:35 – 664. Pyrites for conversion batteries: The effects of cation chemistry on electrochemical performance. **M.M. Butala***, M.A. Lumley, H.A. Evans, R. Seshadri

15:50 – 665. Conversion mechanism of metal oxalates as anode for lithium ion batteries. **H. Oh**, S. Myung

16:05 – 666. Surface coating of electrode/electrode materials for improved electrochemical performance. **J. Xue, X. Dai, Y. Wang, L. Wang, A. Zhou, J. Li***

16:20 – 667. Computer-aided electrolyte development for magnesium ion batteries. **D. Kim***, B. Roy, Y. Lim, Y. Ryu, S. Lee, S. Doo

Hyatt Regency Waikiki
Maloko Blrnm

Nanoporous Materials for Renewable Energy and Sustainability (#266)

Organized by: T. Okubo, S. Qiu, K. Yoon, R. Lobo

Presiding: R.F. Lobo, T. Okubo

13:00 Opening Remarks

13:05 – 668. Layered zeolites: A platform for designing efficient heterogeneous catalysts. **P. Wu***

13:35 – 669. 2D delaminated zeolites as robust and selective catalysts for the sustainable production of industrial chemicals. **C. Ouyang**, R.C. Runnebaum, S.I. Zones, A. Katz

13:55 – 670. Mixed-solvent approach to delaminate layered zeolite precursors. **I. Ogino***, T. Shirobe, S.R. Mukai

14:15 – 671. Nanosized zeolites: Trends in synthesis and applications. **S. Mintova***, A. Khartchenko, H. Awala, V. Valtchev

14:35 – 672. Big or small ZSM-5-crystals: Does size really matter? **P. Losch***

14:55 Coffee Break

15:10 – 673. 3D study of precursor gel morphology and kinetics of EMT zeolite nucleation. G. Melinte, O. Ersen, S. Qiu, S. Mintova, V. Valtchev

15:40 – 674. Enhanced thermal stability and high catalytic performance of selective catalytic reduction of NO_x with NH₃ of high-silica and P-modified AEI zeolites derived from hydrothermal conversion of FAU zeolite in alkylphosphonium hydroxide media. **N. Tsunoda**, T. Sonoda, T. Maruo, Y. Yamasaki, T. Takamitsu, M. Sadakane, T. Sano*

16:00 – 675. Ultrafast and continuous flow synthesis of high silica zeolite SSZ-13 for NO_x removal. Z. Liu, T. Wakihara, k. Oshima, D. Nishioka, E. Shanmugam P, T. Matsuo, T. Takekawa, T. Okubo*

16:20 – 676. Crystalline silica-based material assembled from cage siloxanes modified with silanol groups. N. Sato, Y. Kuroda, H. Wada, K. Kuroda, **A. Shimojima***

16:40 – 677. Mechanism of adsorption-driven structural transition of stack-layer MOFs. **M.T. Miyahara***, S. Hiraide, H. Tanaka

Hyatt Regency Waikiki
Elima

Advances in Microwave Green Chemistry (#360)

Organized by: T. Matsumura, S. Yanagida, R. Varma, K. Jin, S. [ohuchi@bio.kyutech.ac.jp]

Presiding: J. Azuma, H. Shimizu, S. Tsubaki, T. Watanabe

13:00 – 678. Innovative microwave technology for refinery of recalcitrant biomass. **J. Azuma***

13:30 – 679. Application of microwave technology to extraction of essential oils from natural plant products of Afghanistan. N. Faqeryar*, **Y. Mori**, T. Matsumura

13:50 – 680. Application of microwave chemistry for omics analysis. **A. Shiraishi**, T. Yoshimura, S. Ohuchi*

14:05 – 681. Study of molecular efficiency by microwaves in enzymatic reactions: Proposition to define the terms "microwave character" and "microwave effect". **H. Shimizu***, I. Nagashima, J. Sugiyama

14:25 – 682. Application of microwave induced reaction on biomass conversion. **S. Tsubaki***, M. Hiraoka, A. Onda, T. Ueda

14:45 Break

15:05 – 683. Biorefinery study to utilize whole cell wall components for 2nd generation bioethanol and chemicals using microwave processing. **T. Watanabe***

15:35 – 684. Microwave heating mechanism of MBBA in liquid crystalline and isotropic phases as studied by microwave irradiation NMR spectroscopy. **A. Naito***, Y. Tasei, F. Tanigawa, I. Kawamura, T. Fujito, M. Sato

15:55 – 685. Fundamental study of a microwave irradiation structure using transparent post-wall waveguide. **M. Kishihara***, Y. Minamiyama, A. Yamaguchi, Y. Utsumi
16:15 – 686. Electron spin resonance (ESR) spectroscopy as a microwave spectroscopy of free radicals in radical polymerizations. **A. Kajiwara***

16:35 – 687. Incorporation of electrons in 12CaO•Al₂O₃ ceramics by microwave synthesis in nitrogen gas. **H. Visbil***, T. Matsumura, T. Mitani, A. Kajiwara, M. Kishi, K. Hirao

16:50 poster review

Hyatt Regency Waikiki
Mauka Blrnm

Global Strategies for Algal Biomass for Bioenergy and Biorefinery (#407)

Organized by: A. Kondo, J. Yang,
Y. Yoshikuni
Presiding: T. Tanaka

13:00 – 688. Project Green-Eagle: A new biojet fuels initiative in Korea. **M.S. Park**

13:40 – 689. Isopropanol production by metabolically engineered cyanobacteria using a photobioreactor with LED irradiation. **J. Horie***, Y. Kumada, M. Konishi, T. Hanai, Y. Hirokawa, A. Murakami

14:00 – 690. Dynamic metabolic profiling of the marine microalga *Chlamydomonas* sp. JS4 and enhancing its oil production. **T. Hasunuma**, A. Kondo

14:20 – 691. Pyrolysis experiment of lipids in haptophyte algae: Research for biofuel generation. **K. Sawada***, R. Abe, H. Nakamura, H. Araie, I. Suzuki, Y. SHIRAIWA

14:40 Break

14:55 – 692. Engineered microbial platforms for biofuel and renewable chemical production from brown seaweed. **Y. Yoshikuni***

15:35 – 693. Rapid and efficient galactose fermentation by an engineered and evolved *Saccharomyces cerevisiae*. **J. Quarterman, Y. Jin***

* Principle Author

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16:15 – 694. Analysis of macroalgae biomass found around Hawaii for bioethanol production. **B. Yoza**, E. Masutani, S. Masutani
16:35 – 695. Cost-effective harvesting of microalgae from water using polyaluminum chloride coagulant prepared by fresh aluminum hydroxide gels. **X. Tang***, H. Zheng*, C. Zhao*

Friday Evening

Hyatt Regency Waikiki
 Kou Ballroom

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli
 Presiding: S.P. Chaurasia, J.A. Kozinski, R. Sammynaiken

19:00 Opening Remarks-Nanocatalysis for Chemical Production -I
19:02 – 696. Toward a self lighting material for germicidal UV treatment of water. **R. Sammynaiken***
19:22 – 697. Cascade engineered synthesis of γ -valerolactone, 1,4-pentanediol and 2-methyltetrahydrofuran from levulinic acid using novel Pd-Cu/ZrO₂ catalyst in water as solvent. **S. Patankar***, G. Yadav
19:42 – 698. Supercritical water gasification of agricultural and forestry biomass impregnated with nickel nanocatalyst. **S. Nanda***, S.N. Reddy, A. Dalai, J.A. Kozinski*

20:02 – 699. Dehydration of gases in a pressure swing adsorption process using canola meal bioadsorbent. **R. Dhabhai**, C. Niu*, A. Dalai
20:22 – 700. Catalytic performance of La-Ni/Al₂O₃ catalyst for CO₂ reforming of ethanol. **D.N. Vo***, M.B. Bahri
20:40 – 701. Lipase catalyzed esterification of docosahexaenoic acid with lauryl alcohol using immobilized *Pseudomonas cepacia* and *Thermomyces lanuginosus*. **S.P. Chaurasia**, A. Sharma*, A. Dalai

Hawaii Convention Center
 Halls I, II, III

Nanostructured Oxides for Energy Harvesting and Water Splitting (#171)

Organized by: F. Rosei, Z. Wang, E. Diau, A. Vomiero, X. Sun

Poster Session

19:00 – 21:00

702. Vertically-aligned Cu₂ZnSnS₄ nanorod arrays for photoelectrochemical water splitting. **J. Kim**, W. Yang, J. Moon
703. N-doped graphene quantum sheets on silicon nanowire photocathodes for hydrogen production. **U. Sim***, J. Moon*, D. Kim, J. An, J. Kang, K. Nam, B. Hong
704. Low temperature hydrogen production by two-step water decomposition utilizing metal oxides. **M. Okano**, N. Itoh*, T. Sato

Hawaii Convention Center
 Halls I, II, III

Energy Storage in Chemical Bonds: Advances in Chemistry and Materials for Hydrogen Storage (#216)

Organized by: Z. Huang, P. Chen, T. Autrey, Q. Xu, C. Yoon, C. Jensen

Poster Session

19:00 – 21:00

705. Ammonia as a potential chemical hydrogen storage material: Fundamentals and applications. **M. Jeon***, S. Nam, J. Han, C. Yoon
706. Photochemical hydrogen evolution mediated by iron(II) complex with ortho-phenylenediamine. **T. Matsumoto**, H. Chang*
707. Formic acid dehydrogenation using metal nanoparticle catalysts. **N. Tsumori***, M. YADAV, Q. ZHU, Q. XU

708.

Structures formed by para- and ortho-H₂ on MgO(100). **D.B. Jack***, A. Sadeghifar
709. Hydrogen sorption by transition metal modified B-N materials. **Y. Yasuzawa**, Y. WATANUKI, N. Nishimiya*, T. Toyama, Y. Kojima

710.

Study on higher order structure change of NBR rubber with different acrylonitrile contents at high-pressure hydrogen exposure by FTIR spectroscopy. Y. Itoh*, R. Naganuma, T. Kawai, H. Fujiwara, S. Nishimura

711.

Study on the effect of high pressure hydrogen on the higher order structures of NBR rubber materials cross-linked by sulfur and peroxide by using FT-IR spectroscopy. Y. Itoh*, K. Okano, T. Kawai, H. Fujiwara, S. Nishimura

712.

Syntheses, structures, and properties of alkali and alkaline earth metal complexes with o-phenylenediamine. **J. Ishii**, M. Wakizaka, T. Matsumoto, H. Chang

713.

Synthesis of nickel-loaded catalysts from various nickel precursors and investigations on their catalytic activities. T. Nakae, T. Kamegawa*

714.

Development of bimetallic Fe-Ni NPs supported on CeO₂ for hydrogen production from chemical hydrogen storage materials. T. Taga, K. Mori, H. Yamashita*

715.

Theoretical and experimental evidence of graphene supported metal clusters as a potential hydrogen storage material. K. Takahashi*, Y. Wang, S. Isobe, S. Ohnuki

716.

Quantum nature of H₂ in microporous storage materials. **J. D'Arcy***, L. Lindoy, S. Kolmann, M. Jordan

717.

Metal hydride based thermal energy storage systems for high performance concentrating solar power plants. C. Corgnale, B. Hardy, R. Zidan, T. Motyka, J.A. Teprovich, P.A. Ward, B. Peters

718.

Novel nanoconfinement approach of metal hydrides for hydrogen storage applications. M. Sofianos, D. Sheppard, D. Silvester, T. Jensen, C. Buckley*

719.

On the hydrogenation kinetics of N-ethylindole over a supported Ru catalyst. Y. Dong, M. Yang, Z. Yang, H. Cheng*

720.

Phase transitions of tetra-n-butylammonium bromide hydrate enclosing gas molecules. Y. Jin*, M. Kida, J. Nagao

721.

Pincer catalysts for the reversible dehydrogenation of liquid organic hydrogen carriers. H.T. Sartain*

722.

Proton-coupled redox processes of tris-o-benzoquinolinium(FeII) complex. R. Yamamoto, M. Wakizaka, T. Matsumoto, H. Chang*

723.

Recent developments in hydrogen storage materials using carbon nanomaterials. P.A. Ward*, J.A. Teprovich, R.N. Compton, V. Schwartz, G. Veith, R. Zidan

724.

Homo- and hetero-geneous iridium catalysts and their applications in CO₂ hydrogenation. S. Yoon*, K. Park, G. Hariyanandam

725.

Hydrogen sorption and desorption behaviors of metal-carbon composites prepared by various synthesis methods. T. Kaneko, Y. WATANUKI, T. Toyama, Y. Kojima, N. Nishimiya*

726.

Science and technology of hydrogen in energy storage and conversion devices. J.A. Teprovich, P.A. Ward, A. Washington, H. Colon-Mercado, s. greenway, P. Jena, R. Zidan

727.

Hydrogen sorption by transition metal modified CN compound. K. Yokochi, Y. WATANUKI, T. Toyama, Y. Kojima, N. Nishimiya*

728.

Investigation of hydrogen storage and release mechanisms on lithium hydride-polyaniline composite. S. Tsurumi, M. Mizoguchi, A. Yoshida*, W. Ueda

729.

Investigation of Pd nanoparticles supported on zeolites for hydrogen production from formic acid dehydrogenation reaction. M. Navlani-García, M. MARTIS, D. Lozano-Castelló, D. Cazorla-Amorós, Y. Kuwahara, K. Mori, H. Yamashita*

730. Lowering of hydrogen desorption temperatures and reduction of cost of Zr/Fe alloys for practical applications. Y. WATANUKI, T. Toyama, Y. Kojima, N. Nishimiya

731. Low temperature decomposition of ammonia as a hydrogen carrier. A. Oshima, T. Nakayama, T. Sato, N. Itoh*

732. Low-temperature decomposition using a tube-wall and membrane reactor for hydrogen production from ammonia as hydrogen carrier. Y. Kikuchi, T. Sato, N. Itoh*

733. Main-group metal catalysed dehydrocoupling of amine-boranes. H.R. Simmonds, R.J. Less, D.S. Wright*

734. Fluorine-substituted metal hydrides for thermal energy applications. T. Humphries, D. Sheppard, M. Rowles, V. Sofianos, C. Buckley

735. Correlation between stability and mobility of hydrogen occluded in hydrogen storage alloys. S. Hasegawa, Y. WATANUKI, T. Toyama, Y. Kojima, N. Nishimiya

736. Design of plasmonic Pd/Ag catalyst for efficient hydrogen production from ammonia borane. P. Verma, M. Wen, K. Fuku, Y. Kuwahara, K. Mori, H. Yamashita*

737. Electrochemical synthesis of ammonia from water and nitrogen for carbon-free renewable energy carrier. H. Yoon*, J. Kim, C. Yoo, S. Han

738. Dehydrocoupling reactions of main group elements using aluminium based catalysts. L.K. Allen, R. Garcia-Rodríguez, D.S. Wright*

739. Toward the synthesis of magnesium boranates. P. Nguyen, E. Sadeghmojhaddam, M. Chong, J. Yang, C.M. Jensen*

740. Exploring high hydrogen storage performances of lithium alanate by adding different nitrides. Y. Wang, L. Li, Y. Wang, L. Jiao, H. Yuan

741. Formic acid dehydrogenation over Pd/(Ce_xM_yO_{2-d}C₂N₄): Influence of added Ce_xM_yO_{2-d} (M = Cu, Pr, Sm, and Gd) promoter on catalytic activity. M. Ridwan, R. Tamarany, J. Lee, S. Nam, J. Han, C. Yoon

742. Hawaii Convention Center

Halls I, II, III

Nanoporous Materials for Renewable Energy and Sustainability (#266)

Organized by: T. Okubo, S. Qiu, K. Yoon, R. Lobo

Presiding: R.F. Lobo, T. Okubo, S. Qiu, K. Yoon

Poster Session

19:00 – 21:00

742. Ammonia decomposition assisted by membrane reactor: Comparison between silica membrane and palladium membrane. S. Uematsu*, Y. Makino, R. Hayakawa, M. Miyamoto, Y. Oumi

743.

Gradual wet-etching of a 3D cubic mesoporous silica thin film. M. Kobayashi, K. Susuki, Y. Kuroda, H. Wada, A. Shimojima, K. Kuroda

744.

Zeolite capsule catalyst for one-step middle isoparaffin synthesis via Fischer Tropsch synthesis: Growth of H-MOR shell encapsulating fused iron core. G. Yang*, Q. Lin, Y. Yoneyama, H. Wan, N. Tsubaki*

745.

Influence of Si distribution in framework of SAPO-34 membranes on vapor permeation performance in acetic acid dehydration. A.M. Ataher*, M. Matsukata*, M. Seshimo, s. ishiguro

746.

Ethanol direct synthesis from dimethyl ether and syngas on the combination of noble metal impregnated zeolite with Cu/ZnO catalyst. Q. Wei, P. Lu, G. Yang, Y. Yoneyama, N. Tsubaki*

747.

Synthesis of AlPO₄-34 membranes and its water/acetic acid separation performances. M. Seshimo, s. ishiguro, A. Ahmed, M. Matsukata

748.

Ni-based bimodal pore catalysts modified by nanoparticles for enhanced CO₂ methanation. P. Zhu, Q. Chen, G. Yang, Y. Yoneyama, N. Tsubaki*

749.

Water oxidation on mesoporous Ta₃N₅ photocatalysts under visible light. L. GUO*

750.

Polymer sol-gel composite inverse opal catalyst support. X. Zhang, G. Blanchard

751.

Facile synthesis of yolk-shell photocatalyst encapsulating titania within a hollow silica sphere and assessment of its photocatalytic activity. Y. Sumida, Y. Kuwahara, H. Yamashita*

752.

Dehydration of sorbitol to isosorbide in water over high-silica zeolites. R. Otomo, J.N. Kondo, T. Tatsumi, T. Yokoi*

753.

Oxidation of benzene over iron-bipyridine complexes encapsulated in metal cation-exchanged zeolite. Y. Miyake, K. Takiguchi, S. Yamaguchi, H. Yahiro

754.

Catalytic activity of copper(II)-terpy complexes encapsulated into Y-type zeolite. S. Yamaguchi*, A. Suzuki, H. Yahiro

755.

Implementing Indonesian natural resources for synthesizing hierarchically porous ZSM-5 at low temperature. G.T. Kadja, V. Fabiani, R.R. Mukti

756.

Catalytic conversion of guaiacol over Pt loaded nanoporous materials. Y. Park, H. Kim, J. Jeon

757.

Novel synthesis of PAN/PVDF composites based microporous carbons by steam activation for enhancing CO₂ capture and CO₂/N₂ separation. Y. Heo, M. Lee, H. Yang, Y. Choi, S. Lee, D. Jeon, T. Kim, Y. Han, S. Park*

758.

Selective synthesis of light olefins from methanol over nano-sized MFI aluminofeरrosilicate. T. taniguchi, Y. Nakasaka, T. Tago, T. Masuda

759.

Synthesis of zeolite RHO membrane. M. Sakai, M. Tanji, M. Matsukata*

760.

Novel metallosilicate Beta zeolite: Synthesis, characterization, and catalytic application of W-containing Beta zeolite. R. Kosugi, R. Otomo, M. Yoshioka, J.N. Kondo, T. Yokoi*

761.

Construction of nanoporous poly(organosiloxane) networks from various siloxane-based building units. S. Seo, W. Chaikittilip, T. Okubo

762.

Accurate measurement of solid acidity by automatic IRMS-TPD analyzer. S. Suganuma*, Y. Murakami, K. Kanai, N. Katada

763.

Synthesis of highly crystalline AFX-type zeolite by using bulky and rigid diquat molecules as a structure-directing agent. N. Nakazawa, S. Inagaki, Y. Kubota*

764.

Nanoporous hematite structures for efficient water splitting. J. Jang*, H. Ahamadoss, S. Ryu*

765.

Ionic conductivity of nanocomposites formed with mesoporous metal oxides and LiClO₄. S. Matsushita*, H. Kai, Y. Tsushima, K. Inumaru*

766.

Fabrication and morphology control of thin films of conjugated nanoporous polymers. T. Umeda*, W. Chaikittilip, T. Okubo

767.

Fabricating novel MgO-based adsorbent for CO₂ capture at elevated temperature. Y. Li, M. Wan, Y. Wang, J. Zhu*

768.

Effect of boron content in the CON-type aluminosilicate zeolite on the activity in the MTO reaction. M. Yoshioka, T. Yokoi*, T. Tatsumi

* Principle Author

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769. Selective oxidation of bulky sulfides to sulfoxides over Ti-containing mesoporous silica nanospheres. **Y. Wang**, R. Otomo, J.N. Kondo, Y. Kon, T. Yokoi*

770. Immobilization of Ru complexes on organic ligands in periodic mesoporous organosilicas and catalytic application for selective oxidation of alkane. **N. Ishito**, K. Hara*, Y. Maegawa, S. Inagaki, A. Fukuka

771. Chemical vapor deposition of silica on pelletized HZSM-5 for shape-selective disproportionation of toluene into benzene and para-xylene. **D. Mitsuishi**, S. Suganuma*, N. Katada, Y. Araki

772. Selective dealkylation of alkyl naphthalene on silica monolayer catalyst. **Y. Kawaguchi**, S. Suganuma*, N. Katada

773. Enhancement of catalytic activity for disproportionation of toluene by loading Ni on ZSM-5. **A. Okuda**, S. Suganuma*, N. Katada

774. Preparation of transition metal oxides in forms of thin-film on SBA-15. **A. Tsuji**, T. Yokoi, J.N. Kondo*

775. Novel route for the synthesis of nitrogen doped hollow carbon spheres. **Y. Wang**, H. Zou, R. Wang*, Z. Zhang, S. Qiu*

776. Comparative study of nano-sized and hierarchical micron-sized SAPO-34. **X. Chen**, J. Gilson, V. Valtchev

777. One-pot synthesis of hollow organo-silica nanoparticles with tunable interior void size and exterior shell thickness using silica nanospheres as templates. **N. Koike**, Y. Fukada, S. Seo, W. Chaitkittisup, A. Shimojima, T. Okubo*

778. Photo-assisted decomposition of Ru nanoparticles on the fullerenes-introduced mesoporous silica and its catalytic application. **K. Nakatsuka**, Y. Kuwahara, K. Mori, H. Yamashita*

779. Mechanochemical effect for hydrothermal synthesis of Sn substituted MFI-type silicates. **M. Sakaguchi**, H. Kobayashi, M. Nakaya, A. Muramatsu*

780. Exploration of the effect of titania and zirconia based catalyst for catalytic cracking reaction of heavy oil. **H. Kondoh**, K. Tanaka, N. Hasegawa, Y. Nakasaka, T. Tago, T. Masuda

781. Low temperature oxidation of ethylene over Pt nanoparticles in mesoporous silica. **T. Yokoya**, K. Hara, S. Ahmed, A. Fukuka*

782. Alternative method for preparing heteroatom-rich zeolites: Utilization of composites prepared through mechanochemical treatment for the crystallization. **T. Iida**, T. Okubo, T. Wakihara*

783. Co(OH)₂ nanosheets coupled with carbon nanotube arrays grown on Ni mesh for high-rate asymmetric supercapacitors with ideal capacitive behavior. **T. Peng**, H. Wang, X. Wang*

784. Thin layer of cerium oxide coated on SBA-15 mesoporous silica. **J.N. Kondo**, A. Ishikawa, T. Yokoi

785. High oxidation activity of Ti-incorporated silica catalysts derived by grafting of titanium(IV) acetylacetone. **N. Tsunoi***, Y. Yagenji, M. Fukuda, Y. Ide, M. Sadakane, T. Sano*

786. Redox active metal-organic frameworks (MOFs) as high performance cathode active materials for lithium batteries. **Z. Zhang***, H. Yoshikawa, K. Awaga

787. Adsorption removal of small amount of ammonia contained in ammonia decomposed gas for HFCV. **A. Ojima**, T. Sato, N. Itoh*

788. Effect of addition of alcohols into the synthesis gel for ZSM-5 on the structural and catalytic properties. **T. Biligetu**, R. Otomo, J.N. Kondo, T. Yokoi

Hawaii Convention Center
Halls I, II, III

Advances in Microwave Green Chemistry (#360)

Organized by: T. Matsumura, S. Yanagida, R. Varma, K. Jin, S. [ohuchi@bio.kyutech.ac.jp]
Presiding: J. Fukushima, Y. Mori, S. Ohuchi

Poster Session

19:00 – 21:00

789. Application of circularly polarized microwave to asymmetric synthesis. **K. Imaeda***, K. OHTAKE, T. YAMADA

790. Vlsmeyer formylation of aromatic compounds by using microwaves. **T. SUZUKI***, K. TANEMURA

791. Characteristics of the microwave induced flames on the stability and emissions. **E. Lee***, Y. Jeon

792. Microwave irradiation effects for Finkelstein reactions of ferrocene derivatives. **Y. Makabe***, Y. Okada

793. Microwave irradiation effects for esterification reactions of ferrocene. **M. Tachi**, Y. Okada

794. Analysis of microwave heating processes of 1-(4'-cyanophenyl)-4-propylcyclohexane by *in situ* microwave irradiation NMR spectroscopy. T. Yamakami, I. Kawamura, T. Fujio, K. Ushida, M. Sato, A. Naito, Y. Tasei*

795. Molecular mechanism of separation process on microwave assisted extraction and distillation. **M. Abe**, A. Watanabe, N. Iwashashi, S. Ohuchi*

796. Study on resistance of thermophilus under microwave irradiation. **S. Yoshimoto**, R. Nakama, S. Ohuchi*, K. Minekishi

797. Application of microwave heating for fermentation technology. **W. Nagayoshi**, R. Nakama, S. Nakayama, A. Shiraishi, N. Iwashashi, S. Ohuchi*

798. Study of microwave output dependence on enzymatic reaction under microwave irradiation. **F. Aoki**, K. Haraguchi, A. Shiraishi, S. Ohuchi*

799. Optimal microwave output in microbial cultivation. **R. Nakama**, W. Nagayoshi, A. Shiraishi, T. Yoshimura, T. Kodama, S. Ohuchi*

Saturday Morning

Hyatt Regency Waikiki

Kou Ballrm

Integrated Biomass Refinery by Precisely Designed Heterogeneous Catalysts (#54)

Organized by: A. Fukuka, A. Katz, H. Liu
Presiding: A. Fukuka, A. Katz

8:00 – 800. Pyrolysis oil model compound deoxygenation on molybdenum-modified platinum surfaces and supported catalysts. **A. Robinson**, J. Hensley, J. Medlin*

8:15 – 801. Development of metal carbide and nitride nano-catalysts for bio-oil upgrading. **D.A. Ruddy**, F. Baddour, C. Nash, M. Griffin, J. Hensley, J. Schadie

8:30 – 802. Support and promoter effects on hydrocarbon production from bio-oil upgrading over Pt-based catalysts. Z. He, M. Hu, X. Wang*

8:45 – 803. Hydrodeoxygenation of guaiacol over silica-supported copper phosphide catalysts. **P. Khemthong***, C. Geantet, P. Afanasyev, E. Puzenat, N. Viriyapornkul, K. Faungnawakij

9:00 – 804. Kinetic and spectroscopic studies of catalytic mechanisms: Hydrodeoxygenation of biomass feedstocks on transition metal phosphides. **T. Oyama**, A. Iino, A. Cho, P. Bui, K. Bando, A. Takagaki, R. Kikuchi

9:40 – 805. Synthesis of jet fuel range cycloalkanes with cyclopentanone and butanal derived from lignocellulose. **N. Li**, J. Yang, Y. Cong, A. Wang, X. Wang, T. Zhang*

9:55 – 806. Catalyst and process development for hydrotreating of biomass pyrolysis oil. **H. Wang***, S. Lee, D. Anderson, R. Taha, Z. Abdulla

10:10 – 807. Biomass-derived saturated and unsaturated lactones: Mechanistic insights on ring-opening, integrated fermentation, and catalytic processing. **M. Haider**, S. Gupta, N. Sinha, R. Arora, I. Alam

10:25 – 808. Integrated refinery of renewable feedstocks by multitasking heterogeneous catalysts. **K. Kandel**, I.I. Slowing*

10:45 – 809. Plug flow continuous reactor system for rapid conversion of cellulose to glucose using oxygenated carbon catalyst. **A. Shrotri**, H. Kobayashi, A. Fukuoka*

11:00 – 810. Bimetallic catalysts and solvent effects in catalytic conversion of biomass to fuels and chemicals. **J.A. Dumesic***

Hyatt Regency Waikiki
Ekahi

Nanostructured Oxides for Energy Harvesting and Water Splitting (#171)

Organized by: F. Rosei, Z. Wang, E. Diau, A. Vomiero, X. Sun

8:00 – 811. Semiconducting nanostructured metal oxide thin films for high-performance perovskite solar cells. **W. Wu**, F. Huang, D. Chen, Y. Cheng, R.A. Caruso*

8:20 – 812. Oxide materials for dye-sensitized and perovskite solar cells. **P.C. Chen***

8:50 – 813. BaTiO₃ perovskite oxides as an efficient bifunctional oxygen electrocatalyst. **G. Wu***

9:10 – 814. Ceramic injection moulding of Ni-YSZ anode-supported solid oxide fuel cells. **N. Chuankrerkkul***, M. Meepho

9:30 coffee break

10:00 – 815. Development of semiconductor quantum dot sensitized solar cells. **Y. Tachibana***

10:30 – 816. Fabrication of dye-sensitized solar cells using anthocyanin and chlorophyll. **J. Uddin**, A.D. Ward

10:50 – 817. Understanding structural disorder: From engineering new materials to reactivity in natural systems. **R.K. Hocking***, H. King, S. Chang, A. Hesson

11:10 – 818. Photoelectrochemistry and surface science of doped hematite catalysts: from fundamental to applied research. **P. Zhao***

11:30 – 819. Revisiting electronic structure of N⁺, H⁻, and (N, H)-doped TiO₂ based on spin-polarized self-interaction-corrected density functional theory calculations. **Y. Kim***, J. Choi

Hyatt Regency Waikiki
Makai Blrm

Artificial Photosynthesis: Photo-induced Water Splitting (#193)

Organized by: R. Abe, K. Domen, A. Kudo, T. Meyer, J. Lee

Presiding: R. Abe, K. Domen, K. Maeda

8:00 – 820. Water oxidation under visible light using valence band controlled oxy-nitride photocatalysts. **H. Kato***, M. Kobayashi, M. Kakhana

8:15 – 821. Highly selective water oxidation on tungsten oxide (IV) photocatalyst particles having controlled rectangular shapes. **O. Tomita**, S. Nitta, Y. Matsuta, K. Takagi, S. Hosokawa, M. Higashi, R. Abe*

8:30 – 822. Photocatalytic water oxidation over PbCrO₄ with 2.3 eV band gap in IO₃⁻/I redox mediator under visible light. **Y. Miseki***, O. Kitao, K. Sayama

8:45 – 823. Development of photocatalyst plates for Z-scheme water splitting and the factors determining their activity. **Q. Wang**, T. Hisatomi, Q. Jia, A. Kudo, T. Yamada, K. Domen*

9:00 – 824. Visible-light-driven Z-scheme water splitting using tungstic acid as oxygen-evolving photocatalyst. **H. Suzuki**, M. Higashi, R. Abe

9:15 – 825. Heterogeneous photocatalysis: New ideas and methodologies toward efficient water splitting. **K. Maeda***

9:45 Break

10:00 – 826. Photocatalytic water oxidation at the semiconductor-aqueous interface: GaN, ZnO and the GaN/ZnO alloy.

J.T. Muckerman*, M.Z. Ertan,

N. Kharache, M.S. Hybertsen

10:30 – 827. Nanoporous gallium zinc oxynitride photocatalyst for overall water splitting. **B. Adeli**, F. Taghipour*

10:45 – 828. Preparation of nanosheet p-n junction using NiO and Ca₂Nb₂O₁₀ nanosheets and its photocatalytic activity. **S. Ida**, H. Hagiwara, T. Ishihara

11:00 – 829. Use of silicon nanoparticles as photosensitizers for a noble-metal free artificial photosynthesis system. **C.N. Virca**, C. Radlinger, J. Lohmolder, T. McCormick*

11:15 – 830. Light-intensity and particle-size dependence of heterogeneous photocatalytic oxidation of water. **S. TAKEUCHI***, M. Takase, B. Ohtani

11:30 – 831. Photocatalytic hydrogen evolution from aqueous methanol solution using mixed-valence Sn₃O₄ under visible light irradiation. **T. Tanabe***, M. Hashimoto, A.J. Jeevagan, T. Gunji, S. Kaneko, H. Abe, F. Matsumoto

11:45 – 832. Silver phosphate/single wall carbon nanotube composite with enhanced photoactivity and stability under visible light irradiation. **V. Kalousek***, R. Yabunaka, M. SAKAI, Y. Takaguchi, K. Ikeue

Hyatt Regency Waikiki
Maloko Blrm

Nanoporous Materials for Renewable Energy and Sustainability (#266)

Organized by: T. Okubo, S. Qiu, K. Yoon, R. Lobo

Presiding: S. Qiu, K. Yoon

8:00 – 833. Study of structural effects via anodic aluminum oxide as a novel inorganic separator for lithium ion batteries. **Y. Ahn**, Y. Yang, Z. Yin, H. Kim, S. Cho, J. Yoo, Y. Kim*

8:20 – 834. Sustainable carbon materials derived from biomass as platinum-free catalysts for the oxygen reduction reaction in fuel cells. **M. Titirici***, K. Preuss, A. Marinovic

8:40 – 835. Pd nanoparticles encapsulated in hollow titaniosilicate nanospheres as an ideal nanoreactor for one-pot oxidation reaction. **Y. Kuwahara***, T. Ando, H. Yamashita

9:00 – 836. Structure, adsorption free energy, and spectroscopy of ethanol in HZSM-5. **M. Lee**, K. Alexopoulos, M. Reyniers, V. Glezakou, R. Rousseau*

9:20 – 837. New insights into the disproportionation of *n*-propylbenzene and isopropylbenzene catalyzed by zeolites. **Y. Byun***, S. Cha*, K. Lee, I. Nam, S. Hong

9:50 Coffee Break

10:05 – 838. Catalysis for sustainable production of acrylic acid: Potassium-ion exchanged zeolite catalysts for gas-phase dehydration of lactic acid. **B. Yan**, A. Mahmood, Y. Liang, B. Xu*

10:25 – 839. Biomass catalytic fast pyrolysis using hierarchical ZSM-5 zeolites. **D. Gamliel**, L. Wilcox, N. Nguyen, S. Du, G.M. Bollas, J. Valla*

10:45 – 840. Friedel-crafts acylations of furans on lewis-acid-containing zeolites. **M. Koehle**, R.F. Lobo

11:05 – 841. MSE-type zeolite as an efficient catalyst for dimethyl ether-to-olefin reaction. **S. Park**, S. Inagaki, **Y. Kubota***

* Principle Author

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11:25 – 842. Small pore molecular sieve catalysts. **M.E. Davis**

Hyatt Regency Waikiki
Elima

Advances in Microwave Green Chemistry (#360)

Organized by: T. Matsumura,
S. Yanagida, R. Varma, K. Jin,
S. [ohuchi@bio.kyutech.ac.jp]
Presiding: K. Ohta, M. Sato,
N. Shinohara, Y. Wada

8:00 – 843. Synthesis of carbon nanotubes by microwave energy. **K. Ohta***,
T. Nishizawa, T. Nishiguchi, Y. Chino,
R. Shimizu, Y. Hattori, S. Inoue,
M. Katayama, K. Mizu-uchi, T. Kono
8:30 – 844. Theoretical hypothesis on chemical reactions and phase transitions in dense matters with first order fluctuations in Maxwell-Boltzmann velocity distribution. **M. Sato***

8:50 – 845. Study on microwave absorption property of metal particles by electromagnetic simulation. **N. Shinohara***,
S. Arimasa, K. Kashimura, T. Mitani

9:20 – 846. Frequency dependence of oxygen emission of TiO_{2-x} particles by microwave heating. **K. Kashimura**, T. Mitani, N. Shinohara

9:40 – 847. Microwave special effects observed for interfaces. **Y. Wada***,
E. Suzuki, M. Maitani, D. Mochizuki

10:10 Break

10:25 – 848. Reduction enhancement of copper oxides via selective heating, internal heating, and cleavage of Cu-O bond by microwave magnetic-field irradiation. **J. Fukushima***, H. Takizawa

10:45 – 849. Microwave non-thermal acceleration of photoinduced electron transfer from CdS quantum dots to bipyridinium derivatives. **F. Kishimoto***, D. Mochizuki, T. Imai, M. Maitani, E. Suzuki, Y. Wada

11:05 – 850. Science outreach of microwave technology in Japan. **S. Tsubaki**, N. Asahi, I. Ikenaga, S. Ohuchi, S. Kato, M. Nishioka, Y. Homma, T. Matsumura, T. Mitani, Y. Wada

11:25 – 851. Aurora in Pyrex glass tubes and molecular modeling of microwave plasma. **S. Yanagida***, T. Kida, T. Matsumura

11:45 closing remark

Hyatt Regency Waikiki
Mauka Blrnm

Global Strategies for Algal Biomass for Bioenergy and Biorefinery (#407)

Organized by: A. Kondo, J. Yang,
Y. Yoshikuni
Presiding: Y. Yoshikuni

8:00 – 852. Microalgae-based CO₂ reutilization and biorefineries. **J. Chang***

8:40 – 853. Kinetic study of nutrients recovery from microalgae in hydrothermal liquefaction. **C. Fushimi***, M. Kakimura, T. Tateishi, T. Tanaka

9:00 – 854. Microalgae extraction the use of solvent mixtures CO₂:MeOH. R. Lee, P.G. Jessop, P. Champagne

9:20 – 855. Life cycle analysis of energy balance and CO₂ reduction in green oil production process by microalgae.

M. Matsumoto*, T. Tanaka, H. Togashi, H. Hasegawa

9:40 Break

9:55 – 856. Biorefinery of seaweeds for biofuels, chemicals, and feed. **A. López Contreras**

10:35 – 857. Valuable substances production using marine biomass wastewater. **Y. Okamura***, H. Takahashi, S. Suzuki, M. Okawachi, T. Nomura, T. Aki, Y. Nakashimada, Y. Matsumura

10:55 – 858. Modified CO₂-switchable cellulose nanocrystal and its application in microalgal harvesting for biofuel production. S. Ge, H. Wang, P. Champagne*, M. Cunningham, P.G. Jessop

11:15 – 859. Development of alginate fuel cells for biorefinery of macroalgae. **H. Yoshioka***, H. Toake, H.T. VU, E. Tamia

Saturday Afternoon

Hyatt Regency Waikiki
Kou Ballrm

Integrated Biomass Refinery by Precisely Designed Heterogeneous Catalysts (#54)

Organized by: A. Fukuoka, A. Katz, H. Liu
Presiding: J.N. Beltramini, Y. Wang

13:00 – 860. Direct catalytic conversion of cellulose to light naphthalene. **M. Dusselier***, B. Op de Beeck, B. Sels

13:15 – 861. Design of dual functional polymeric solid acid catalysts for biomass hydrolysis and dehydration. **X. Qian***, V. Ahn, R. Wickramasinghe

13:30 – 862. Catalytic transformations of cellulose and its derived carbohydrates into organic acids. W. Deng, Q. Zhang, Y. Wang*

14:10 – 863. Hydrolysis of lignocellulosic biomass by biomass-derived carbon catalyst. **H. Kobayashi**, A. Fukuoka*

14:25 – 864. Understanding the adsorption and depolymerization of polysaccharides on carbon surface. **P. Chung**, A. Katz, J. Chu

14:40 – 865. On route to carbon catalyst design for polysaccharide depolymerization. A.T. To, P. Chung, A. Charmot, A. Katz

15:00 – 866. Dehydration synthesis of valuable chemicals from biomass-derived materials. **A. Yamaguchi***, O. Sato, N. Mimura, M. Shirai

15:15 – 867. Environmentally benign hydrogenation of biomass-derived compounds with supported metal catalysts and water solvent. **M. Shirai***, Y. Nagasawa, K. Yoshida, H. Nanao, T. Sasaki, O. Sato, A. Yamaguchi

15:30 – 868. Conversion of delignified Indonesian rice hulk to levulinic acid using hierarchical Mn/ZSM-5 catalyst. **Y.K. Krisnandi***, A. Agnes, D.A. Nurani, R. Pertwi

15:45 – 869. Tailored one-pot production of furan-based fuels from fructose in ionic liquid-containing biphasic solvent system. **C. Li, H. Cai, B. Zhang, T. Dai, A. Wang, T. Zhang**

16:00 – 870. Single metal atom catalyst: How does it help in biomass conversion. **N. Yan***

16:20 – 871. New route to biomass-derived terephthalic acid using Lewis acid molecular sieve catalysts. **M.E. Davis**

Hyatt Regency Waikiki
Ekahi

Nanostructured Oxides for Energy Harvesting and Water Splitting (#171)

Organized by: F. Rosei, Z. Wang, E. Diau, A. Vomiero, X. Sun

13:00 – 872. Nanostructured ceria by pulsed laser deposition for hydrogen and methane electro-oxidation. **S.M. Haile**, W. Jung

13:30 – 873. Solution processable inorganic-organic hybrids for solar cells and water splitting. **M. Loi***

14:00 – 874. Nanostructured oxides and organic-inorganic hybrid materials for photocatalytic hydrogen production. A. Beltram, T. Montini, M. Melchionna, M. Prato, P. Fornasier*

14:20 coffee break

14:50 – 875. Electrochemical impedance spectroscopy and pH-dependent kinetics of α -Fe₂O₃ ultrathin films for photoelectrochemical water splitting. **J. Moir**, N. Sohelnia, G. Ozin

15:10 – 876. Evaluation of different types of tungsten oxide nanomaterials for photoelectrochemical water splitting. **S. Hilaire**, M. Niederberger

15:30 – 877. Synthesis of Cu_xZn_ySn_zS-oxide nanowalls on carbon cloth and the application in photoelectrochemical water splitting. **Y. Pei**, C. Shen, J. Chiu, Y. Tai*

Hyatt Regency Waikiki
Makai Blrnm

Artificial Photosynthesis: Photo-induced Water Splitting (#193)

Organized by: R. Abe, K. Domen,
A. Kudo, T. Meyer, J. Lee
Presiding: T. Meyer, L. Sun, M. Yagi

13:00 – 878. Solar water splitting in dye sensitized photoelectrosynthesis cells.

T. Meyer, L. Alibabaei, K. Brennaman, B. Sherman, M. Sheridan, A. Nayak, D. Ashford, S. Roy

13:30 – 879. Electrochemical instability elucidation of metal oxide adsorbed phosphonate-derivated Ru(II) poly-pyridyl complexes. D. Harrison*, M. Raber, J. Hyde, K. Hanson, A. Vanucci, A. Lapides, L. Alibabaei, M. Norris, T. Meyer

13:45 – 880. Dye-sensitized NiO as p-type photocathode for photovoltaic and solar fuel devices. **L. Hammarström***, A. Brown, L. Zhang, L. d'Amario, L. Antila, J. Föhlunger, P. Ghamsarov, S. Maji, S. Pullein, G. Boschloo, H. Tian, S. Ott

14:00 – 881. Creation of novel heterogeneous nickel complex catalyst for visible-light-driven H₂ evolution from water. **H. Kakudo**, K. Mori, H. Yamashita*

14:15 – 882. Accumulation of charge at molecular acceptors through excitation of molecular dyes: One step closer to effective solar water splitting using molecules. H. Chen, W. Gaieck, S. Breen, J. Siu, A. Rouzmehr, S. Ardo

14:30 – 883. Two-electron water activation on earth abundant aluminum porphyrins as a key-step for artificial photosynthesis.

F. Kuttassev, S. Mathew, S. Sagawa, D. Yamamoto, S. Onuki, Y. Nabatani, H. Tachibana, H. Inoue*

14:45 Break

15:00 – 884. Artificial photosynthesis: Photoelectrochemical (PEC) cells for water splitting based on molecular catalysts.

L. Sun, Y. Gao, F. Li

15:30 – 885. Thin film transition metal phosphide and sulfide catalysts for applications in photoelectrochemical water splitting.

T.R. Hellstern, J.D. Benck, J. Kibsgaard, R. Britto, C. Hahn, T.F. Jarailimo*

15:45 – 886. Mesoporous IrO₂ thin film for highly efficient electrocatalytic water oxidation toward artificial photosynthesis.

D. Chandra, N. Abe, D. Takama, K. Saito, T. Yui, M. Yagi

16:00 – 887. Multifunctional NiO_x coated small band-gap semiconductors for efficient and stable solar driven water oxidation.

K. Sun*, F.H. Saadi, Y. Kuang, X. Zhou, B.S. Brunschwig, C.W. Tu, N.S. Lewis

16:15 – 888. Designing 2D covalent organic frameworks for photocatalytic hydrogen evolution.

F. Haase, V. Vyas, B.V. Lotsch*

16:30 – 889. Well-defined and nanostructured IrO_x water splitting electrocatalysts for efficient solar fuel production in acidic PEC and PEM environments.

P. Strasser*

16:45 – 890. Photonic nanostructures for efficient solar water splitting. **L. Zhang***

Hyatt Regency Waikiki
Maloko Blrnm

Nanoporous Materials for Renewable Energy and Sustainability (#266)

Organized by: T. Okubo, S. Qiu, K. Yoon, R. Lobo
Presiding: S. Qiu, K. Yoon

13:00 – 891. Propellane polycyclic structures as a springboard to new SDA for zeolites: The discovery of a new high silica zeolite.

S.I. Zones*, D. Xie, M.M. Olmstead, A. Liu, K. Ghiasi

13:30 – 892. Structure-directing effect of pipерazine revealed by reverse temporal evolution processes. **W. Yan***

13:50 – 893. Cyclophosphazene bridged mesoporous organosilicas for CO₂ capture and Cr(VI) removal. P. Rekha, V. Sharma, P. Mohanty*

14:10 – 894. New class of ZSM-5 catalyst: Synthesis and catalytic performance of ZSM-5 with the distribution of Al atoms in the framework controlled. **T. Yokoi***, T. Biligetu, R. Otomo, J.N. Kondo, T. Tatsumi

14:30 – 895. Al-rich beta zeolites. Distribution of Al atoms in the framework and related protonic and metal-ion species.

J. Dedecek*, P. Szazma, S. Sklenak, B. Wichterlova, E. Tabor, P. Klein, V. Pashkova

14:50 Coffee Break

15:05 – 896. Hydrocarbon trap and more on aluminum-rich beta zeolites for clean-up technology of automobiles. **M. Ogura***

15:35 – 897. Synthesis of Pt/C catalysts with a high sintering resistance using activated carbon xerogels as the support. K. Satoh, T. Tsuchiya, S. Iwamura, I. Ogino, S.R. Mukai*

15:55 – 898. Facile synthesis of metal/metal oxide nanoparticles inside nanoporous carbon matrix (M/MO@C) through morphology-preserved transformation of metal-organic framework for energy applications. W. Bak, H. Kim, W. Yoo*

16:15 – 899. Selectively-tuned rare earth adsorption in hybrid mesoporous sorbents: The critical role of ligand design.

J. Florek, A. Mushtaq, E. Juère, F. Fontaine, D. Larivière, F. Kleitz*

16:35 – 900. Hydrothermal synthesis of porous self-regulating humidity materials.

Z. Jing, J. Fan, Y. Zhang

Hyatt Regency Waikiki
Elima

Bridging Homogeneous and Heterogeneous Catalysis in Biorefining of Lignin (#405)

Organized by: F. Wang, F. Toste, H. Xie, D. Argyropoulos, R. Rinaldi, R. Baker
Presiding: D. Argyropoulos, H. Xie

13:00 Session kickoff

13:05 – 901. The biorefinery industry need to refine lignin prior to use in a way similar to crude. **D. Argyropoulos***

13:45 – 902. Biobased-organic electrolytes lignin: Separation, structural elucidation, and application. **H. Xie**, C. Peng, X. Yu, Z. Zhao

14:05 Break

14:15 – 903. Electrocatalytic energy upgrading of lignin model compounds to fuels and chemicals: A green chemistry imperative. **J. Jackson**, C. Saffron, C. Lam, M. Garedew, P. Hao

14:35 – 904. Catalytic conversion of sugar-cane bagasse lignin into value-added products: A strategy for separating and recycling ionic liquids. **X. Li***

14:55 – 905. Lipoxygenase: A new versatile oxidative enzyme in lignin upgrade.

C. Crestini*, H. Lange

15:15 – 906. Supercritical water-induced lignin reactions: A structural and quantitative assay. **Y. Liu***, J. weikun, L. gaojin

15:45 Break

15:45 – 907. Catalytic conversion of lignin into aromatics by tungsten- and rhenium-based catalysts. **T. Zhang***, C. Li, B. Zhang, A. Wang

* Principle Author

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Hyatt Regency Waikiki
Mauka Ballrm

Global Strategies for Algal Biomass for Bioenergy and Biorefinery (#407)

Organized by: A. Kondo, J. Yang,
Y. Yoshikuni
Presiding: M.S. Park

13:00 – 908. Development of biorefinery from microalgae and cyanobacteria.
A. Kondo

13:40 – 909. Drop-in-fuel production from alkenone-producing marine haptophyte algae. **Y. SHIRAIWA***, H. Araie, Q. Shi, Y. Tsuji, T. Kotajima, Y. Hanawa, I. Suzuki, H. Nakamura, K. Sawada

14:00 – 910. Photosynthetic hydrogen formation in *Chlamydomonas reinhardtii*.
F. Mamedov, A. Basu, S. Styring, A. Volgusheva

14:20 – 911. Investigation of kinetics of cultivation of low temperature tolerant *Chlorella vulgaris* for lutein production and recovery. **A. Bassi***

14:40 Break

14:55 – 912. Construction of genome designed yeasts for direct assimilation of macroalgae by synthetic biology.

T. Takagi*, Y. Sasaki, K. Motone,

H. Morisaka, K. Kuroda, M. Ueda

15:35 – 913. Achieving high glycogen production rates in the marine cyanobacterium, *Synechococcus* sp. PCC 7002 through metabolic engineering.

A. Markley*, B. Pfleger

15:55 – 914. RNA-based gene regulators for controlling gene expression in cyanobacteria. **Y. Sakai**, I. Sakamoto, C. Shono, S. Kawai, K. Abe, K. Sode, K. Ikebukuro*

16:15 – 915. Bacterial metagenomes as potential resources for isolation of biorefinery enzymes in brown macroalgae degradation. **T. Mori***, M. Takahashi, Y. Yumiko, T. Shibata, T. Takagi, R. Tanaka, H. Miyake, K. Kuroda, M. Ueda, H. Takeyama

16:35 Closing remark

Saturday Evening

Hawaii Convention Center
Halls I, II, III

Integrated Biomass Refinery by Precisely Designed Heterogeneous Catalysts (#54)

Organized by: A. Fukuoka, A. Katz, H. Liu
Presiding: A. Fukuoka, M. Yabushita

Poster Session

19:00 – 21:00

916. Production of phenolic compounds from lignin by two step process.

Y. Nakasaka*, R. Konishi, Y. Kawamata,

T. Yoshikawa, Y. Koyama, T. Tago,

T. Masuda

917. Effect of basic property of Co-loaded catalysts on hydrodeoxygenation of guaiacol. **M. Iwaki***, N. Ikenaga

918. Hydrogenation of alkylphenol over supported metal catalysts in water solvent.

Y. Nagasawa, H. Nanao, O. Sato,

A. Yamaguchi, M. Shirai*

919. Synthesis of high density aviation fuel with cyclopentanol derived from lignocellulose. N. Li, **X. Sheng**, G. Li, W. Wang, J. Yang, Y. Cong, A. Wang, X. Wang, T. Zhang

920. Synthesis of jet-fuel range aromatic hydrocarbons by the hydrodeoxygenation of isophorone over $\text{MoO}_x/\text{SiO}_2$. N. Li, **F. Chen**, W. Wang, A. Wang, Y. Cong, X. Wang, T. Zhang*

921. Synthesis of renewable diesel or jet fuel range alkanes with 2-methylfuran. N. Li, **G. Li**, A. Wang, Y. Cong, X. Wang, T. Zhang*

922. Designing a new $\text{CO}/\text{ZrO}_2-\text{SiO}_2$ bimodal catalyst for jet-fuel direct synthesis from a CO_2 -containing syngas via Fischer-Tropsch synthesis. **J. Li**, G. Yang, Y. Yoneyama, N. Tsubaki*

923. Catalytic conversion of xylose to furfural in water and simultaneous extraction with supercritical carbon dioxide. **O. Sato***, A. Yamaguchi, Y. Masuda, Y. Kiyouzumi, N. Mimura, E. Kato, M. Shirai

924. Study of the effect of model size and solvation on the formation of levoglucosan. L. Aebersold, J. Henry, B. Leja, D. Wang, A. Seitz, **J. Song***

925. Conversion of cellulose to n-hexane or hexanol over $\text{Ir}-\text{ReO}_x/\text{SiO}_2$ catalyst combined with acid. **S. Liu**, M. Tamura, Y. Nakagawa, K. Tomishige

926. Hydrolysis of woody biomass by air-oxidized carbon catalyst. **K. Techikawa**, H. Kobayashi, H. Kaiki, A. Fukuoka

927. Adsorption and hydrolysis of cellulose molecules on activated carbon catalysts. **M. Yabushita**, H. Kobayashi, J. Hasegawa, K. Hara, A. Fukuoka*

928. Dehydration of sorbitol to isosorbide over β -zeolites. **H. Yokoyama**, H. Kobayashi, M. Yabushita, B. Feng, A. Fukuoka*

929. Furural synthesis from bamboo powder with CHA-type zeolite and water solvent. **K. Yoshida**, H. Nanao, O. Sato, Y. Kiyouzumi, A. Yamaguchi, M. Shirai*

930. Selective synthesis of 2-methyltetrahydrofuran from levulinic acid using solid acid-supported Pt-Mo bimetallic catalyst. **K. Togo**, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa, K. Kaneda*

931. Effect of Sn addition on the conversion reaction of ethanol to the C4 compounds over $\text{Ru}/\text{Al}_2\text{O}_3$ catalyst. **S. Ishikawa**, A. Yoshida, J. Nakazawa, S. Hikichi, S. Naito

932. Hydrogen production by aqueous phase reforming reaction of acetic acid over supported ruthenium catalysts. **T. Nozawa**, A. Yoshida, J. Nakazawa, S. Hikichi, S. Naito*

933. Sustainable catalytic conversions: Production of organic acids from inedible-biomass resources over heterogeneous catalysts. **H. Choudhary**, S. Nishimura, K. Ebizani*

934. Development of precisely designed heterogeneous catalysts for valorization of biomass-derived feedstock. **T. Mizugaki**, Z. Maeno, T. Mitsudome, K. Jitsukawa, K. Kaneda*

935. Highly selective transesterification of glycerol to monoacetylglycerol using heterogeneous base catalysts. **T. Morita**, Z. Maeno, T. Mitsudome, T. Mizugaki, K. Jitsukawa, K. Kaneda*

936. Bifunctional Mo-V-O/ZSM-5 catalysts for direct oxygenation of glycerol to acrylic acid. **T. Hisazumi**, S. Suganuma*, N. Katada

937. Synthesis of bio-based thiophene derivatives with supported ionic liquids in a fluidized bed reactor. **P. Filippouli**, Z. Zhang, J. Wilton-Ely, P. Fennell, J.P. Hallett*

938. Ni based alloy catalysts for chemoselective hydrogenation of unsaturated carbonyls. **S. Shimazu***, W. Putro, R. Rodiansono, T. Hara, N. Ichikuni

939. High-performance Cu/SiO_2 catalyst for ethylene glycol synthesis via dimethyl oxalate hydrogenation. **G. Liu**, P. Ai, G. Yang, Y. Yoneyama, N. Tsukuba*

940. Conversion of volatiles produced from polyacrylonitrile-based carbon fiber manufacture over Ni/dolomite catalyst. **Q. Sun***, M. Ye, J. Chen, Z. Wu

Hyatt Regency Waikiki
Kou Ballrm

Nano Catalysis for Clean Energy and Environmentally Friendly Chemical Production (#81)

Organized by: A. Dalai, N. Abatzoglou, B. Davis, A. Uddin, J. Kozinski, G. Yadav, A. Tavasoli

Presiding: Y. Chin, K.K. Pant

19:00 Opening Remarks-Nanocatalysis for Chemical Production -II

19:02 – 941. Oxidative steam reforming of bio-ethanol over multifunctional $\text{Ni}/\text{Al}_2\text{O}_3-\text{CeO}_2-\text{ZrO}_2$ catalyst. **T. Mondal**, M. Sajhani, **K.K. Pant***, A. Dalai

19:22 – 942. Treatment of phenol in water using microwave assisted advanced oxidation processes. A. Verma, **V. Meda**, A. Dalai

19:40 – 943. Visible light driven transformation of aliphatic alcohols to corresponding esters in O_2 under mild conditions. **Q. Xiao***, H. Zhu*

20:00 – 944. Catalytic consequences of reactant size and local site confinement for aldehyde deoxygenation on solid Brønsted acid catalysts. **F. Lin**, **Y. Chin**

20:20 – 945. Synthesis, characterization, and catalytic applications of K-CoRhMo catalysts supported over carbon nanohorns (CNHs) and its by-products (OCP & OCP_f) for the HAS reaction. **P.E. Boahene**, A. Dalai*, R. Sammynaiken

20:40 – 946. Selective hydrogenation of α,β -unsaturated aldehydes to unsaturated alcohols over metal oxide-modified Ir catalysts. **M. Tamura**, Y. Nakagawa, K. Tomishige

Hawaii Convention Center
Halls I, II, III

Artificial Photosynthesis: Photo-induced Water Splitting (#193)

Organized by: R. Abe, K. Domen, A. Kudo, T. Meyer, J. Lee

Poster Session

19:00 – 21:00

947. Preparation of gold nanoparticle/layered semiconductor hybrids and their application to photocatalytic hydrogen evolution. **M. Eguchi***, K. Maeda

948. Effects of composition and surface modification on PEC properties of $\text{In}(\text{Ga})\text{Se}_2$ photoanodes. **H. Kaneko**, T. Minegishi, K. Domen*

949. Photoelectrochemical properties of SrNb_2O_7 photoanodes based on highly crystalline particles using flux methods. **M. Kodera**, H. Urabe, T. Hisatomi, M. Katayama, T. Minegishi, K. Domen*

950. Fabrication of Ta_3N_5 photoanodes for solar water splitting by thin film transfer process. **C. Wang**, T. Hisatomi, T. Minegishi, T. Yamada, J. Kubota, K. Domen*

951. Synthesis of a series of bismuth mixed anions compounds and their application to photocatalytic water splitting and photovoltaic systems. **H. Kunioku**, A. Nakamura, M. Higashi, R. Abe*

952. Effect of visible-light-induced oxidation of water using Al porphyrin adsorbed on semiconductor. **S. Onuki**, D. Yamamoto, S. Mathew, F. Kuttassery, Y. Nabetani, H. Tachibana, H. Inoue*

953. La-Ti oxysulfides as a photoelectrode for water splitting. **G. Ma**, J. Liu, T. Hisatomi, T. Minegishi, H. Nishiyama, M. Katayama, T. Yamada, K. Domen*

954. Photophysical and electrochemical study of tin porphyrins as molecular catalyst for artificial photosynthesis. **A. Thomas**, D. Yamamoto, Y. Nabetani, S. Onuki, H. Tachibana, H. Inoue*

955. Tailoring the redox properties of silicon porphyrins for water activation. **S.N. Remello**, T. Hirano, D. Yamamoto, S. Onuki, Y. Nabetani, H. Tachibana, H. Inoue*

956. Direct fabrication of Ta_3N_5 photoanode via nitridation of NaTaO_3 precursor film prepared by hydrothermal-electrochemical method. **S. Osada**, C. Izawa, T. Watanabe

957. Synthesis of SrNb_2O_7 photocatalyst by flux assisted nitridation with co-nitriding agent. **Y. Hirano**, H. Ebato, T. Watanabe

958. Utilization of cage-type ligands for photochemical and oxygen-converting transition metal complexes. **Y. Funahashi***, K. Hara, S. Yonaga, K. Nagata, T. Hatanaka

959. Application and analysis of protection layers for photoinduced water oxidation in alkaline media. **M.F. Licherman***, S. Hu, B. Richter, E. Crumlin, S. Axnanda, M. Favaro, W. Drisdell, Z. Hussain, T. Mayer, B.S. Brunschwig, N.S. Lewis, Z. Liu, H. Lewerenz

960. Enhanced water oxidation on metal oxynitrides photocatalysts under visible light by using polyoxometalates as co-catalysts. **Y. Iwase**, O. Tomita, M. Higashi, R. Abe*

961. Paddlewheel-type dirhodium tetracarboxylate complexes as catalyst for photochemical hydrogen evolution from water. **Y. Kataoka***, N. Yano, T. Kawamoto, M. Handa

962. Highly efficient photochemical reduction of water using anchor-shape dinuclear rhodium complexes. **N. Yano***, Y. Kataoka, T. Kawamoto, M. Handa

963. Efficient photochemical production of hydrogen in aqueous solution by simply incorporating a water-insoluble hydrogenase mimic into hydrogel. **T. Yu**, **Y. Li***

964. Rhodium-doped barium titanate semiconductor photocatalyst prepared by a hydrothermal method for hydrogen evolution under visible light. **S. Nishioka***, O. Ishitani, K. Maeda

965. Overall water splitting on a restacked nanosheet photocatalyst with highly dispersed noble metal nanoparticles. **T. Oshima***, O. Ishitani, K. Maeda

966. Robust artificial photosynthetic catalyst made in situ from QDs and metal salts for efficient hydrogen evolution. **Z. Li***, X. Fan, C. Tung, L. Wu*

967. Preparation of heterostructured $\text{ZnSe}/\text{AgInS}_2$ nanoparticles and their photocatalytic properties. **M. Kishi***, T. Kameyama, S. Kuwabata, T. Torimoto

968. High performance photoelectrolysis tandem cell system for solar hydrogen production. **H. Nishiyama**, Y. Kuang, N. Sato, H. Kobayashi, M. Zhong, Q. Jia, T. Minegishi, T. Hisatomi, T. Yamada, K. Domen*

969. Solar powered hydrogen production using conjugated polymer films. **P. Fortin***, G. Suppes, S. Holdcroft

970. Exploring the possibilities of guest-host supramolecular systems of earth abundant metal incorporated molecular catalyst for artificial photosynthesis.

S. Mathew, F. Kuttassery, D. Yamamoto, S. Onuki, Y. Nabetani, H. Tachibana, H. Inoue*

971. Photocatalytic reduction of CO_2 over nanocomposites of mesoporous silica and SrTiO_3 nanocubes. **T. Ohashi***, Y. Miyoshi, K. Katagiri, K. Inumaru*

972. Ta_3N_5 -based photoanodes for solar-light-driven water splitting. **M. Zhong***, Y. Sasaki, H. Nishiyama, T. Yamada, K. Domen

973. Importance of the surface passivating ligand of CdSe quantum dots for photocatalytic hydrogen evolution. **K. Sawaguchi**, A. Kobayashi*, M. Yoshida, M. Kato*

974. Effect of Sr vacancies and substitutionals on the bandstructure of SrNb_3O_7 : A DFT analysis. **M. Kaneko***, G. Giorgi, K. Yamashita

975. Red-light induced all-solid-state Z-scheme using silver as a redox shuttle. **R. Kobayashi**, K. Kurihara, S. Tanigawa, T. Takashima, H. Irie*

976. Grafting cocatalyst onto zinc rhodium oxide/silver/defective silver antimonate hetero-junction photocatalyst to enhance water-splitting activity. **S. Matsumoto**, R. Kobayashi, H. Irie*

977. Photocatalytic activity of perovskite oxides containing tetravalent lanthanide ions. **Y. Yoshida**, N. Taira*, M. Ota

978. Synthesis and photoelectrochemical properties of antimony-based ternary semiconductors containing halogen anions. **M. YABUCHI**, M. Higashi, R. Abe*

* Principle Author

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Global Strategies for Algal Biomass for Bioenergy and Biorefinery (#407)

Organized by: A. Kondo, J. Yang,
Y. Yoshikuni

Poster Session
19:00 – 21:00

- 979.** Analysis of composition and antioxidative properties of phlorotannins isolated from Japanese *Eisenia* and *Ecklonia* species. **T. Shibata***, K. Nagayama*, T. Saitoh, R. Tanaka, H. Miyake, Y. Tamaru, S. Kawaguchi, M. Ueda
- 980.** Intracellular and extracellular time-course proteome analyses of *Clostridium cellulovorans* grown on xylan. **S. Aburaya***, J. Shin, K. Esaka, H. Morisaka, K. Kuroda, M. Ueda
- 981.** Molecular breeding of yeasts for platinum reduction. **R. Ito***, H. Hashimoto, K. Kuroda, M. Ueda
- 982.** Development of in vivo methylation system for gene-modification of cellulolytic bacterium, *Clostridium cellulovorans*. **J. Shin***, A. Ishitaka, K. Kuroda, M. Ueda
- 983.** Molecular breeding of yeast for assimilating xylan from marine biomass. **Y. Sasaki***, T. Takagi, H. Morisaka, K. Kuroda, M. Ueda
- 984.** Construction of “glucose formation platform” using cellosome-producing bacterium *Clostridium cellulovorans*. **T. Inamori***, A. Ishitaka, S. Aburaya, H. Morisaka, K. Kuroda, M. Ueda
- 985.** Molecular breeding of yeasts for utilization of a marine polysaccharide laminarin. **K. Motone***, T. Takagi, H. Morisaka, K. Kuroda, M. Ueda
- 986.** Regulatory mechanisms for expression of cellosomal and non-cellosomal genes in *Clostridium cellulovorans*. T. Ishikawa*, R. Tanaka, T. Shibata, K. Kuroda, M. Ueda, Y. Tamaru, H. Miyake*
- 987.** Creation of new cellosome-producing strains for next generation biorefinery. **A. Hiramatsu***, K. Kuroda, M. Ueda, Y. Tamaru, H. Miyake*
- 988.** Development of a transformation system for the mesophilic cellosome-producing bacterium *Clostridium cellulovorans*. **M. Okada***, H. Miyake*
- 989.** Identification of cellosomal enzymes for the construction of cellosomes from *Clostridium cellulovorans*. **C. Nagaya***, G. Ishikawa*, R. Tanaka, T. Shibata, K. Kuroda, M. Ueda, Y. Tamaru, H. Miyake*
- 990.** Characterization of novel alginate lyases of *Falsihydrobacter* sp. alg1 isolated from brown algae. **M. Takahashi**, T. Mori*, R. Tanaka, T. Shibata, S. Chow, K. Kuroda, M. Ueda, H. Takeyama
- 991.** Energy-saving lipid extraction from wet microalgae by low-boiling-point solvent dimethyl ether at room temperature. **H. Kanda***, R. Hoshino, K. Murakami, M. Ogawa, S. Machmudah, W. Diono, M. Goto
- 992.** Alkane production by genetically engineered marine cyanobacterium *Synechococcus* sp. NRBG 15041c. **Y. Ito**, Y. Liang, N. Nakunaka, T. Yoshino, T. Tanaka*
- 993.** Genetic engineering for the overproduction of polyhydroxybutyrate in cyanobacteria. S. Hondo, M. Takahashi, T. Osanai, M. Matsuda, T. Hasunuma, A. Tazuke, Y. Nakahira, S. Chohman, M. Hasegawa, **M. Asayama***
- 994.** Overproduction of alkane as biofuel from an engineered cyanobacterium under heterotrophic culture condition. **H. Fukuda**
- 995.** Control the self-aggregation of cyanobacteria by regulating pilus gene. **A. Ito**, M. Nakamura, K. Abe, K. Kojima, S. Ferri, K. Sode*
- 996.** Engineering of a wide dynamic range green-light regulation system for gene expression in *Synechocystis* sp. FCC 6803. **C. Shono**, K. Abe, I. Sakamoto, K. Ueno, Y. Sakai, K. Sode, K. Ikebukuro*

997. Improving photoautotrophic growth by maintaining a fixed growth pH and a sufficient inorganic carbon. **B. Nguyen***, B.E. Rittmann

998. Synthesis of CdSe nanoparticles by using a low concentration of cadmium ions and the apoeroferritin of marine pennate diatoms. **M. Yamane**, I. Yamashita, K. Iwahori*

999. Quantitative analysis of pH stress response in maltose-excreting *Chlorella* using transcriptomic profiling. **V. Natarajan**, K. Coster, B. Barney

1000. Characterization of the cold-tolerant oleaginous diatom, *Mayamaea* sp. JPCC CTDA0820 as potential source for biodiesel production. **D. Nojima**, K. Ikeda, M. Matsumoto, Y. Maeda, T. Yoshino, T. Tanaka*

1001. Alkenone and transcriptome analysis of the response to cold temperature in the marine haptophyte alga, *Emiliania huxleyi*. **H. Arai***, M. Baba, T. Kotajima, I. Suzuki, Y. SHIRAIWA

1002. Diversity of hydrocarbons produced by alkenone-producing haptophyte algae. **H. Nakamura***, H. Arai, K. Sawada, I. Suzuki, Y. SHIRAIWA

1003. Development of fucose fuel cell for biorefinery of macroalgae. **H.T. VU**, H. Yoshikawa, H.Q. Le , H. Toake, E. Tamiya*

1004. Effect of salinity on methanogenic propionate degradation by acclimated marine sediment-derived culture. **T. Miura**, A. Kita, Y. Okamura, T. Aki, Y. Matsumura, T. Tajima, J. Kato, Y. Nakashimada*

1005. Analysis of anaerobic alginate degradation mechanism in bacterial consortium. **A. Kita***, T. Miura, Y. Okamura, T. Aki, Y. Matsumura, T. Tajima, J. Kato, N. Nishio, Y. Nakashimada

1006. Direct analysis via mass spectrometry of products from hydrothermal pretreatments of glucose. **P. Duangkaew**, S. Inoue, T. Aki, Y. Nakashimada, Y. Okamura, T. Tajima, Y. Matsumura*

1007. Decomposition reaction of D-(+)-mannose under hydrothermal condition. **R. Mohamad**, T. Aki, Y. Nakashimada, Y. Okamura, T. Tajima, Y. Matsumura*

1008. Squalene production by marine bacterium in wastewater derived from algal biomass. **S. Suzuki**, M. Suemitsu*, Y. Takahashi*, M. Matsumoto*, T. Aki*, Y. Nakashimada*, Y. Matsumura*, Y. Okamura*

1009. Screening of triacylglycerol producing bacteria for reducing propionic acid. **M. Okawachi**, M. Suemitsu*, M. Matsumoto*, T. Aki*, Y. Matsumura*, Y. Nakashimada*, H. Takahashi*, Y. Okamura*

1010. Efficient production of biodiesel from marine alga, *Scenedesmus* sp. from acidic in situ transesterification process. **H.Y. Lee***, W.Y. Choi, D.H. Kang

1011. Hydrothermal liquefaction of macro algae to value added hydrocarbons. **R. Singh**, B.B. Krishna, B. Thallada*

1012. Enhancement of biomass productivity in marine oleaginous diatom *Fistulifera solaris* by silencing of fucoxanthin chlorophyll a/c binding protein gene. **T. Yoshino**, C. Takahashi, M. Muto, Y. Liang, Y. Maeda, T. Tanaka

1013. Dynamic oil body generation in the marine oleaginous diatom *Fistulifera solaris* JPCC DA0580 following in response to nutrient limitation revealed by morphological and lipidomic analysis. **Y. Liang**, K. Osada, Y. Maeda, T. Yoshino, C. Bowler, T. Tanaka

1014. Proteome analysis of the oil body-associated proteins in the marine oleaginous diatom *Fistulifera solaris* JPCC DA0580. **Y. Maeda**, D. Nojima, T. Yoshino, T. Tanaka*

1015. Cell-surface display of interactive proteins on the oleaginous diatom *Fistulifera solaris* for biomass harvesting. **T. Tateishi**, Y. Maeda, M. Muto, T. Yoshino, T. Tanaka*

Sunday Morning

Hyatt Regency Waikiki
Kou Ballrm

Integrated Biomass Refinery by Precisely Designed Heterogeneous Catalysts (#54)

Organized by: A. Fukuoka, A. Katz, H. Liu
Presiding: H. Liu, T. Shishido

8:00 – 1016. AuPd bimetallic nanoparticles catalyzed selective oxidation of biomass-based 1,6-hexanediol to 6-hydroxycaproic acid using H_2O_2 oxidant in basic aqueous solvent. **S. Nishimura**, J. Tuteja, H. Choudhary, K. Ebitali*

8:15 – 1017. Lactic acid formation from 1,3-dihydroxyacetone over phosphate/TiO₂ with water-tolerant Lewis acid sites. **K. Nakajima***, M. Hara

8:30 – 1018. Separations in integrated biomass refinery. K. Park, S. Yiaccoumi*, C. Tsouris, A. Borole

8:45 – 1019. Selective dehydrocyclization-cracking of soybean oil using zeolite-alumina composite supported PtNiMo catalysts. **A. Ishihara***, T. Ogiyama, T. Hashimoto, H. Nasu

9:00 – 1020. In-situ spectroscopy studies on surface reactions of biomass-derived oxygenates. **C. Sievers**, G. Foo , J.R. Copeland, J. So

9:20 – 1021. Hydrogenolysis of glycerol over Pt/WO₃/Al₂O₃ catalysts. H. Kobayashi, H. Miura, T. Shishido*

9:35 – 1022. Catalytic behavior of Pd-Re catalyst in glycerol hydrogenolysis to propane diols – effect of Pd precursors. Y. Li, D. He

9:55 – 1023. Development of heterogeneous metal catalysts for the production of biomass-derived chemicals by catalytic hydrogenolysis and hydrogenation. **K. Tomishige***

10:35 – 1024. Rule-based and experiment-coordinated reaction network generation and analysis of coking in catalytic pyrolysis of bio-oil relevant model compounds. S. Du, D. Gamliel, J. Valla, **G.M. Bollas***

10:50 – 1025. Periodic trends and requirements for aqueous phase transfer hydrogeneration of acetic acid on Group VIII metal clusters. J. Shangguan, **Y. Chin**

11:05 – 1026. Selective hydrogenolysis of furfural to 1,2-pentanediol catalyzed by hydrotalcite-supported platinum nanoparticles. **M. Mizugaki**, Y. Nagatsu, Z. Maeno, T. Mitsudome, K. Jitsukawa, K. Kaneda*

11:20 – 1027. Catalytic conversion of cellulose to ethylene glycol: from fundamental discovery to potential commercialization. M. Zheng, J. Pang, A. Wang, **T. Zhang**

Hyatt Regency Waikiki
Ekahi

Nanostructured Oxides for Energy Harvesting and Water Splitting (#171)

Organized by: F. Rosei, Z. Wang, E. Diau, A. Vomiero, X. Sun

8:00 – 1028. Self-assembly formation and contributing factor of epitaxial nano-groove arrays on rock salt structured oxide thin films. **A. Matsuda**, R. Yamauchi, S. Kaneko, M. Yoshimoto

8:20 – 1029. Metal-to-insulator transition studies of vanadium oxide and samarium nickelate thin films for energy devices. **M. Chaker***, N. Emond, B. Torris

8:50 – 1030. Fabrication of abundant Zn vacancies in ZnO for p-type conductivity, room-temperature ferromagnetism and high photocatalytic activity. **L. Pan**, X. Zhang, L. Wang, J. Zou*

9:10 – 1031. Reduced graphene oxide supported nickel, manganese, and cobalt ternary oxide nanocomposite catalysts for oxygen evolution reaction. **R. Miao**, J. He, Z. Luo, W. Song, S. Sub

9:30 coffee break

10:00 – 1032. Synthesis and bacterial resistance of zwittrionic MCM-41 nanostructured materials. **E. Delgado***, F. Villegas, O. Rodriguez, I. Izquierdo, A. Salinas, M. Vallet-Regi, G. Toriz

10:20 – 1033. Effect of phosphate ions for water oxidation using iridium oxide catalysts. **Y. Inaba**, K. Nakamura, T. Kuwabara, T. Yamaguchi, K. Takahashi*

Hyatt Regency Waikiki
Makai Blrm

Artificial Photosynthesis: Photo-induced Water Splitting (#193)

Organized by: R. Abe, K. Domen, A. Kudo, T. Meyer, J. Lee
Presiding: R. Abe, A. Kudo, F. Osterloh

8:00 – 1034. Photocatalytic and photoelectrochemical solar water splitting using reduced graphene oxide-incorporated metal sulfides. **A. Iwase**, K. Iwashina, I. Honma, A. Kudo

8:15 – 1035. Advanced materials manufacturing in solar water splitting technologies. **E.L. Miller***

8:30 – 1036. Computational identification of materials for solar energy conversion including semiconductors for water splitting. **D.S. Ginley***, S. Lany, W. Tumas, V. Stevanovic

8:45 – 1037. Recent progress in wide bandgap chalcopyrite thin film materials development for unbiased photoelectrochemical hydrogen production. **N. Gaillard***, Deangelis, C. Heske, M. Blum, T.F. Jarillo-Herrero, T.R. Hellstern, T. Ogitsu, h. wang

9:00 – 1038. Photoelectrode system for the production of hydrogen and high-value-added oxidation reagents. **K. Sayama***, K. Fuku, Y. Miseki, T. Funaki

9:15 – 1039. Measuring junction potentials at illuminated particle photocatalysts. **F. Osterloh***

9:45 Break!

10:00 – 1040. Electrochemical synthesis of ternary oxide photoelectrodes for use in solar water splitting. **K. Choi**

10:30 – 1041. Durable water oxidation under simulated sunlight using BaTaO₂N photoanodes prepared by particle transfer method. **K. Ueda**, T. Minegishi, T. Hisatomi, M. Katayama, T. Yamada, K. Domen

10:45 – 1042. Silicon based devices for cheap, efficient, and scalable solar water splitting. **W. Smith**

11:00 – 1043. Absorption of light in silicon microwire arrays for photo-electrochemical applications. **M. Dasog**, N.S. Lewis*

11:15 – 1044. Thin film fabrication of BaNbO₂N for photoelectrochemical water oxidation. **M. Katayama**, M. Kodera, R. Tajima, T. Minegishi, J. Kubota, K. Domen

11:30 – 1045. Designing water splitting devices composed of photocatalysts. **T. Yamada***

Hyatt Regency Waikiki
Maloko Blrm

Nanoporous Materials for Renewable Energy and Sustainability (#266)

Organized by: T. Okubo, S. Qiu, K. Yoon, R. Lobo
Presiding: R.F. Lobo, T. Okubo

* Principle Author

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8:00 – 1046. Summary of nanoporous materials research at CSIRO Australia.
M.R. Hill

8:20 – 1047. Redox activity of a nanoporous metal-organic framework MIL-100 for cathode of lithium ion battery.
T. Yamada, K. Masutani

8:40 – 1048. Hierarchical porous prussian blue analog nanocrystals for sodium-ion battery applications.
M. Hu*

9:00 – 1049. Intriguing differences in hydrogen adsorption in CPO-27 materials induced by metal substitution.

M.H. Rosnes, M. Optiz, M. Frontzek, W. Lohstroh, J.P. Emba, P.A. Georgiev, P.D. Dietzel*

9:20 – 1050. Syntheses of hydrothermally stable metal-organic frameworks and their applications to adsorption-driven heat transformation.
Y. Hwang, U. Lee, C. Serre, S.M. Humphrey, J. Chang

9:50 Coffee Break

10:05 – 1051. Development of zeolite membranes for isopropyl alcohol dehydration process.
M. Matsukata*

10:25 – 1052. Hybrid nanoporous materials for acid gas removal.
A. Sayari*

10:45 – 1053. Selective CO₂ capture from humid flue gases and humid atmosphere using a novel microporous coppersilicate.
S.J. Datta, C. Khumnoon, Z. Lee, W. Moon, I. Hwang, K. Yoon*

11:05 – 1054. Supercapacitive swing adsorption of carbon dioxide.
B. Kokoszka, N.K. Jarrah, C. Liu, D.T. Moore, K. Landskron

11:25 – 1055. Light gas separations and storage with MOFs via modeling, synthesis, and pressure induced structural changes.
T. Nenoff*, D. Sava Gallis, M. Parkes, J. Greathouse, M. Rodriguez, K. Chapman

11:55 Closing Remarks

Hyatt Regency Waikiki
Elina

Bridging Homogeneous and Heterogeneous Catalysis in Biorefining of Lignin (#405)

Organized by: F. Wang, F. Toste, H. Xie, D. Argyropoulos, R. Rinaldi, R. Baker
Presiding: R. Baker

8:00 – 1056. Selective, catalytic aerobic C-C bond cleavage of lignin models and extracts.
R. Baker*

8:40 – 1057. Hydroconversion of lignin-derived phenolic and aromatic ether compounds over highly active Ni-Nb-O catalysts.
C. Liang

9:00 Break

9:10 – 1058. Lignosulfonate-based acidic resin for the synthesis of renewable diesel and jet fuel range alkanes with 2-methylfuran and furfural.
S. Li, N. Li, G. Li, A. Wang, Y. Cong, X. Wang, T. Zhang*

9:30 – 1059. Direct and selective hydrolysis of arenols and aryl methyl ethers.
S. Kusumoto, K. Nozaki*

9:50 Break

10:00 – 1060. Hydrodeoxygenation of ethanol organosolv lignin to aromatic hydrocarbons by metal-organic frameworks.
J. Zhou*, w. xing, j. wenchao, g. yanzhu, h. ying, l. haiming

10:20 – 1061. Utilization of lignin isolated using steam process to produce added-value chemicals (L-chems) and drop-in jet fuel (L-fuels).
J. Lavoie*, F. Lemoine, K. Louis

10:40 – 1062. Hydrogenolysis of lignin and lignosulfonate over nickel-based catalysts.
F. Wang

HLTH

Area 10 – Bench to Bedside: Chemistry of Health Care

Tuesday Morning

Sheraton Waikiki
Waialua

Oligonucleotide Therapeutics: From Base Pairs to Bedsides (#8)

Organized by: M. Manoharan, M. Damha, T. Wada
Presiding: M.J. Damha

8:00 Opening remarks

8:05 – 1. Efficient intramolecular decarboxylative process for the cleavage of 2'-O-iminoxyethyl propanoate protecting groups from RNA sequences.
S.L. Beaucage*

8:35 – 2. DNA/RNA heteroduplex oligonucleotide for highly efficient gene silencing.
T. Yokota*

9:05 – 3. GalNAc-conjugated siRNAs as a new paradigm in RNAi therapeutics.
M. Manoharan*

9:35 – 4. Advances in tumor delivery of siRNA: Non-hepatic xenograft, GEMM and PDx Tumor Models and CTNNB1-targeted RNAi.
B.D. Brown*

10:05 Break

10:20 – 5. Taking lessons from nature for the delivery oligonucleotide therapeutics.
A. Levin*

10:50 – 6. Development of polymeric materials for systemic siRNA delivery to solid tumor.
K. Miyata*, K. Kataoka

11:20 – 7. Studies of modified oligonucleotides directed toward nucleic acid drugs.
M. Sekine*

11:50 Closing remarks

Sheraton Waikiki
Waianae

Fragment-based Lead Discovery (#145)

Organized by: D. Erlanson, M. Scanlon, K. Ruan, D. Tanaka, J. Tyndall
Presiding: D. Erlanson

8:00 Introduction - Library design and computational analysis

8:10 – 8. Building confidence for chemistry by utilization of a quality library and a multidisciplinary approach.
J.M. Withka*, M. Boehm, C. Augusto de Oliveira, K.A. Borzilleri, M. Calabrese, N. Caspers, D. Hepworth, R. Kurumbail, A. Morgan, F. Rajamohan, P. Sahasrabudhe, H. Wang, V. Shanmugam Sundaram

8:40 – 9. Challenges in targeting diverse sites.
C. Squire*, Y. Yosaatmadja, S. Fung, L. Ching, J. Flanagan

9:10 – 10. Fragment libraries and their application to a protein-protein interaction target.
G. Chessaar*

9:40 – 11. Binding hot spots, fragment conservation, and druggability.
S. Vajda*, D. Kozakov, D. Hall

10:00 Break

10:10 – 12. Non-ATP competitive inhibitors are selective for PLK1 and target tumors resistant to catalytic site compounds.
C. Micinnes

10:30 – 13. High throughput screening, structure-based, and fragment-based drug discovery: Modern data workflows and analytics.
K. Gregory

10:50 – 14. Hitting it big on small molecular entities: A new way of assessing binding affinity.
C. Detering

11:10 – 15. Can solvent mapping drive optimization of a fragment based campaign for epoxide hydrolase?
G.L. Warren*, A.G. Skillman, J.M. Word, S. Wlodek, H. Kack

11:30 – 16. Importance of hydration thermodynamics in fragment-to-lead optimization.
O. Ichihara*

Royal Hawaiian
Regency II

Spectroscopic Tools for the Treatment of Cancer (#397)

Organized by: N. Miyoshi, B. Wilson, W. Ahn, M. Cherukuri
Presiding: W. Ahn, Y. Okamoto

8:00 – 17. Self-assembled, covalently linked, hollow phthalocyanine nanospheres.
W.S. Ahn*, P. Chaturvedi, Y. Kim, K. Kim, S. Han

8:30 – 18. Relationship between anti-tumor effects of PDT and parameters including light irradiation using talaporfin sodium in vivo model.
Y. Okamoto*, T. Osaki, T. Imagawa, K. Azuma, N. Ito, T. Tsuka, Y. Murahata, T. Kohama, Y. Kawase, H. Iseki, S. Ikuta, Y. Muragaki, S. Kishimoto

9:00 – 19. Cancer cellular specific incorporation of 5-aminolevulinic acid by mitochondrial reactive oxygen species.
H. Matsui, H. Ito, M. Tamura, T. Kaneko, H.P. Indo, H.J. Majima

9:25 – 20. Chlorine e6-folic acid-curcumin conjugate based sono-photodynamic therapy.
P. Chaturvedi*, Y. Kim, S. Han, W.S. Ahn

9:50 Break

10:00 – 21. Clinical progress of photodynamic therapy in the treatment of tumor in China.
H. Qiu*, Y. Gu*, J. Zhang, N. Huang, , Wang, J. Zeng

10:25 – 22. Effect of talaporfin sodium-mediated photodynamic therapy in KLN205 cells and Meth A cells.
T. Osaki*, Y. Hashimoto, K. Azuma, Y. Murahata, T. Tsuka, N. Ito, T. Imagawa, Y. Okamoto, Y. Kawase, H. Iseki, S. Kishimoto, S. Ikuta, Y. Muragaki

10:50 – 23. Development of pH-activatable tetraphenylporphyrin derivatives as photosensitizers for PDT.
H. Horiochi*, R. Kuribara, A. Hirabara, T. Okutsu

11:15 – 24. Three in one: A multifunctional antitumor sensitizer for photodynamic, boron neutron capture and ionized X-rays therapies.
N. Miyoshi*, S.K. Kundu, V. Mandal, M. Sakurai, H. Tanaka, M. Suzuki, V.G. Ol'shevskaya, A.A. Shtil

Sheraton Waikiki
Oahu

Recent Advances in Microfluidics for Radiochemical Synthesis (#416)

Organized by: G. Pascali, Y. Kuge, R. Dam
Presiding: Y. Kuge, G. Pascali, R. van Dam

8:00 Introductory Remark

8:05 – 25. Challenges, benefits, and potential risks of switching to microfluidic chemical synthesis.
P. Watts*

8:40 – 26. Devising flow chemistry protocols to access radiopharmaceuticals.
L.K. Spare, A.M. Krause-Heuer, L. Matesic, I. Greguric, G. Pascali, B.H. Fraser, J. Aldrich-Wright, C. Gordon*

8:52 – 27. Digital radiochemistry on microfluidic chip.
M. Javed, S. Chen, H. Kim, M.E. Sergeev, C. Kim, R. van Dam, P. Keng*

9:27 – 28. Application of microfluidic-based technology toward the synthesis of ¹⁸F-heteraryl silanes for biomolecular labeling.
J.M. Murphy*, C. Waldmann, A. Touvet, R.H. Grubbs

10:02 Morning Break

10:12 – 29. One-flow synthesis of *N*-succinimidyl 4-¹⁸F-fluorobenzoate using a single microfluidic chip.
H. Kimura*, H. Saiki, Y. Hasegawa, Y. Tokuda, M. Ono, E. Ozeki, Y. Kuge, R. Iwata, H. Saji

10:47 – 30. Simple hydrolysis and purification methods for ¹⁸F-MISO synthesis.
N. Abo*, N. Manri, K. Nishijima, F. Feng, N. Kuno, N. Tamaki, Y. Kuge

10:59 – 31. Use of microfluidics in the concentration and formulation of PET tracers.
P.H. Chao*, R. van Dam

11:11 – 32. Development of a microreactor system for syntheses of positron emission tomography: PET imaging probes.
Y. Asano*, S. Togashi, N. Manri, N. Kuno, Y. Ito, H. Tsudome

11:23 – 33. Automation of radiochemistry in microscale volumes.
A. Hsiao*, J. Thompson, A. Crane, M. Gramlich, B. Maraglia, R. van Dam, M.D. Moore*

11:35 – 34. Application of microreactor with split-flow and interflow mixing for synthesis of positron emission tomography (PET) imaging probe.
N. Kuno*, N. Manri, N. Abo, Y. Asano, K. Nishijima, N. Tamaki, Y. Kuge

Tuesday Afternoon

Sheraton Waikiki
Waialae

Oligonucleotide Therapeutics: From Base Pairs to Bedsides (#8)

Organized by: M. Manoharan, M. Damha, T. Wada
Presiding: T. Wada

13:00 Opening Remarks

13:05 – 35. Impact of structure for understanding stability, pairing properties, and activity of chemically modified nucleic acids.
M. Egli*

13:35 – 36. Developing TNA as an artificial genetic polymer for molecular medicine.
J. Chaput*

14:05 – 37. From front loading to affinity maturation: Finding optimal modifications on nucleic acid ligands.
N. Janjic*, J. Carter, J. Rohloff, C. Fowler, B. Ream, G. Wardle, T. Fitzwater, D. Schneider, T. Jarvis, D. Davies, B. Gawande, A. Gelinas

14:35 – 38. New generation PNA analogs for effective cell permeation.
K. Ganesh*

15:05 Break

15:15 – 39. Phosphorodiamidate morpholino oligonucleotides (PMOs): A versatile therapeutic platform.
R. Kole*

15:45 – 40. Sterecontrolled synthesis of boron-containing oligonucleotides as therapeutic agents.
T. Wada*

16:15 – 41. Evaluation and properties of chemically-modified siRNAs.
J. Desauviers*, G. Hagen, B. Peel

16:35 – 42. Creation of the hypoxia-specific oligonucleotide therapeutics system with intracellular environment-responsible peptide ribonucleic acids (PRNAs).
T. Wada*

16:55 Closing Remarks

Sheraton Waikiki
Waianae

Fragment-based Lead Discovery (#145)

Organized by: D. Erlanson, M. Scanlon, K. Ruan, D. Tanaka, J. Tyndall
Presiding: M. Scanlon

13:00 NMR methods

13:00 – 43. Applications of ligand-based NMR spectroscopy in inhibitor discovery.
I.K. Leung, M. Demetriadis, T. Brown Jr, M. Abboud, J.L. Andersson, A.M. Rydzik, A. Khan, E. Flashman, C.J. Schofield*, T.D. Claridge*

* Principle Author

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<http://pacificchem.org/onlineprogram>

13:30 – 44. Binding site identification and fragment optimization using ligand-detected NMR. **S.J. Headley***, D. Garriga, M. Pearce, C. Accurso, S. Bottomley, F. Coulibaly, M. Scanlon

13:50 – 45. Fast structure determination of low affinity protein-ligand complexes from sparse NMR data. **B. MOHANTY***, M. Williams, B.C. Doak, M. Vazirani, O. Ilyichova, W. Bermel, D.K. Chalmers, J. Simpson, G.F. King, M. Mobil*, M. Scanlon*

14:20 – 46. Solid-state NMR investigations of small-molecule binding sites. **S. Matsuo***

14:50 Break

15:00 – 47. Map and Target: A NMR-based method for small molecule binding validation. **D.M. Dias***, C. Spry, M. Sabbah, A. Ciulli, C.F. Geraldes, C. Abell

15:20 – 48. Using a fragment based drug discovery approach for the development of Neisseria DsdB inhibitors. **B. Heras***, R. Smith, M. Scanlon, S.J. Headley

15:50 – 49. Practical aspects of ¹⁹F NMR spectroscopy for fragment-based hit identification. **T. Haselhorst**

16:10 – 50. ¹⁹F NMR: A valuable probe of protein-ligand interactions. **R.S. Norton***

16:30 – 51. Synergistic approaches to fragment based lead discovery: Getting the most out of your fragments. **J.B. Jordan***

Royal Hawaiian Regency II

Spectroscopic Tools for the Treatment of Cancer (#397)

Organized by: N. Miyoshi, B. Wilson, W. Ahn, M. Cherukuri

Presiding: N. Miyoshi, Y. Ogawa

13:00 Introduction

13:05 – 52. Observation of intercellular water dynamics on sub-picosecond timescales by terahertz spectroscopy. **Y. Ogawa***, K. Shiraga, N. Kondo

13:35 – 53. Application of hyperthermia by irradiation of sub-THz wave from a gyrotron and a possibility of combination with photodynamic therapy for cancer.

N. Miyoshi*, S.K. Kundu, V. Mandal, T. Takahashi, T. Idehara

14:05 – 54. "Plasma thermograms": Heat profiles of blood for the detection and monitoring of cancer. **N.C. Garbett***, G.N. Brock, D.J. Fish, A. Kalaiappan, M. Granger-Delacroix, N.C. Allen, D.M. Miller, J.A. Chesney

14:30 Break

14:40 – 55. Raman spectra exploring breast tissues applying support vector machine. **T. Gao**

15:05 – 56. Diagnosis of esophageal cancer in early stage by Raman spectroscopy with various chemometrics techniques.

M. Ishigaki*, Y. Maeda, A. Taketani, A.B. Bibin, R. Ishihara, K. Wongravee, Y. Ozaki, H. Sato

15:30 – 57. FT-IR 3000M for studying the phosphodiester group distribution in some tumor. **B.B. Andriana***, H. Sato, N. Miyoshi

15:55 – 58. Fourier-transform infrared (FT-IR) microscopic imaging for clinical raw tissues. **N. Miyoshi***, Y. Imamura, A.B. Bibin, T. Okoshi, T. Goi, A. Yamaguchi

Sheraton Waikiki
Oahu

Recent Advances in Microfluidics for Radiochemical Synthesis (#416)

Organized by: G. Pascali, Y. Kuge, R. Dam
Presiding: Y. Kuge, G. Pascali, R. van Dam

13:00 Introductory Remarks

13:05 – 59. Microfluidic promises and challenges: "... to GMP or not to GMP, that is the question". **P.A. Salvadori***

13:40 – 60. Ru-catalyzed direct methylation of amines from CO₂ in a microfluidic environment. **M.B. Peterson**, G.J. Perkins*, A. Kallinen, O. Khatib, A. Ung, I. Greguric, G. Pascali

13:52 – 61. Peptide radiolabeling strategies. **J. Sutcliffe**

14:27 – 62. Applications of microfluidics to radiometal based radiopharmaceuticals. **D.E. Reichert***

15:02 Afternoon Break

15:12 – 63. Recent advances in microfluidics. **T.L. Collier**

15:47 – 64. Challenges of producing ^{[18]F}-HBG using continuous flow microfluidics. **L. Matesic***, A. Kallinen, I. Greguric, G. Pascali

15:59 – 65. Microfluidic surface-enhanced electrochemical fluorination. Q. He, R. van Dam, S. Sadeghi

16:11 – 66. Lab-on-a-chip for radiotracer synthesis and quality control. **N. Pamme***

Wednesday Morning

Sheraton Waikiki
Waialua

Oligonucleotide Therapeutics: From Base Pairs to Bedsites (#8)

Organized by: M. Manoharan, M. Damha, T. Wada

Presiding: M. Manoharan

8:00 Opening Remarks

8:05 – 67. Genome and epigenome editing with CRISPR/Cas9 technologies for gene therapy and disease modeling. **C. Gersbach**

8:35 – 68. Recent progress in the development of bridged nucleic acids. **S. Obika***

9:05 – 69. "Smart" delivery systems that open the intracellular target universe. **P. Stayton***

9:35 – 70. Toward the rational design of chemically modified siRNAs endowed with drug like properties. **P. Pushpangadan Indra***

10:05 Break

10:15 – 71. Role of high-purity solvents and reagents in oligonucleotide synthesis: Purity by design. **V. Mohan***

10:45 – 72. Gene silencing using structural variants of small interfering RNAs. **D. Lee***

11:15 – 73. Cyclic nucleotides and bacterial biofilm formation. **T. Yan***, E. Bordeleau, C. Oberc, M. Bell, N. Heidari, J. Li

11:35 – 74. RNA duplex binding molecules as carriers for siRNAs. **R. Iwata***, F. Nakayama, S. Hirochi, K. Sato, Y. Maeda, W. Piao, K. Nishina, T. Yokota, T. Wada*

11:55 Closing Remarks

Sheraton Waikiki
Oahu

Chemistry for Development of Theranostic Radiopharmaceuticals (#11)

Organized by: D. Wilbur, M. Adam, P. Donnelly, Y. Arano, J. Jeong, X. Zhang
Presiding: M.J. Adam, D.S. Wilbur

8:00 Opening Remarks

8:05 – 75. Introduction to theranostic radionuclides. **S.S. Juriszon***

8:35 – 76. Dedpa family of chelates for radio-metals. **M.J. Adam***, C. Orvig, C. Ramogida

9:05 – 77. Imaging and therapeutic possibilities with copper, rhenium, and technetium complexes. **P.S. Donnelly***

9:35 – 78. Cyclam propionates: Stable copper(II) chelates for radiopharmaceutical application. **M. Kubell***, K. Zarschler, J. Pietzsch, H. Stephan, P. Comba

9:50 – 79. Optimizing technetium and rhenium small-molecules for enhanced biological behavior. **A. Mahmood***, T. Uehara, Y. Peng, Z. Akgun, N. Limpa-Amara, A.G. Jones

10:05 Break

10:15 – 80. Design and fabrication of radiolabeled probes for imaging and therapy of tumors. **F. Wang***

10:45 – 81. Immuno-PET of epithelial ovarian cancer: The promise of a magic bullet. **F. Wuest**

11:15 – 82. Phospholipid ethers: A broad spectrum cancer imaging and therapy delivery platform. **J.P. Weichert***, A. Pinchuk, J. Kuo, J. Jeffery, R. Zhang, J. Grudzinski, B. Titze, M. Longino

11:45 – 83. Development of enzyme mediated imaging and therapy (EMIT) as a novel theragnostic agent for metastatic prostate cancer. **J. Kronauge**, J. Jenson

Sheraton Waikiki
Waianae

Fragment-based Lead Discovery (#145)

Organized by: D. Erlanson, M. Scanlon, K. Ruan, D. Tanaka, J. Tyndall

Presiding: K. Ruan

8:00 Fragment finding and characterization

8:00 – 84. REFLI: A chemical strategy for the rapid elaboration of fragment hits into more potent lead compounds. **M. Scanlon***

8:30 – 85. Use of thermodynamic tools in the early stages of fragment-based drug discovery. **J.M. Caaveiro***, T. Mitani, K. Tsumoto*

8:50 – 86. New techniques, old techniques, and new ideas: Fragment screening revisited. **T.S. Peat**, L.A. Woods, O. Dolezal, B. Ren, J. Ryan, S. Poulsen*

9:20 – 87. Fishing for fragments to complement known binders. **D. Erlanson***

9:45 Break

9:55 – 88. Fragments and covalent inhibitors targeting macrophage migration inhibitor factor for inflammatory disease and cancer. **J. Tyndall***, L. Kok, M.T. Rutledge, C.T. Vo, A.B. Gamble, S.M. Wilbanks, M. Hampton

10:25 – 89. Combining acrylamide warheads with fragment based drug discovery to find a new class of glutaredoxin targeted antibiotics. **T.C. Leeper***, D.L. Morris, R. Khatri

10:45 – 90. Genetically-encoded fragment-based discovery. **R. Derra***

11:10 – 91. Is there anything fragments can't do? Fragment discovery against a new target class. **E.R. Zartler**, T. Messick, K. Malecka, P. Lieberman

11:30 – 92. Recent experiences of fragment-based drug design at Astellas. **T. Niimi***

Hawaii Convention Center
Halls I, II, III

New Antibacterial Agents (#236)

Organized by: J. Finn, J. Palmer, H. Arimoto

Poster Session

10:00 – 12:00

93. PNIPAM nanospheres grafted to polypropylene fabric for thermally controlled release of bacteriophage.

H.J. Hathaway*, P. Perez-Esteban, D. Alves, K. Ouadi, J. Bean, A. Jenkins, M. Sutton

94. Arrival of imidazo[1,2-b]thiazole-carboxyamides as potent inhibitors of *Mycobacterium tuberculosis*. **G.C. Moraski***, P. Miller, J.R. Anderson, S. Cho, S. FRANZBLAU, M.J. Miller*

95. Water-soluble, selective Fe-binding polymer as synergic agent for antibiotic enhancement. **M. Bierenstiel***, T. Ang, B.E. Holbein

96. Synthesis and evaluation of flavonol derivatives as potent anti-MRSA agents. **K. Sasaki***, A.. Hossian, Y. Wang, Y. Zamami, T. Kuroda

97. Thioethers – active against *Mycobacterium tuberculosis*. **M. Konaklieva***, R. Kusovskiy, K. Arora, H. Boshoff, C. Barry III

98. Synthesis and antibacterial evaluation of macrocyclic diarylheptanoid derivatives. **H. Lin, D. Bruhn, M. Maddox, R. Lee, R. Lee, D. Sun**

99. Exploration of the mechanism of action and structure-activity relationship for a new class of quinazolinone antibiotics.

R. Bouley, M. Kumarasiri, Z. Peng, D. Ding, L. Otero, W. Song, M.A. Suckow, V.A. Schroeder, W.R. Woiter, E. Lastochkin, N.T. Antunes , H. Pi, S. Vakulenko, J.A. Hermoso, M. Chang*, S. Mobashery

100. Synthesis, characterization, biological activity and cytotoxicity of copper complexes of imine-pendant derivatives of *ortho*-(S-methylthio) aniline. **M. Bierenstiel***, K. Ckless

101. Development of novel infection inhibitors targeting iron-uptake pathways against group a streptococcus. **M. Hoshino***, J.M. Caaveiro, S. Nagatoishi, I. Nakagawa, K. Tsumoto

102. Penicillin-binding protein 4 of *Pseudomonas aeruginosa*, a nexus for the induction of β -lactam antibiotic resistance. **J.F. Fisher***, M. Lee, D. Hesk, B. Blazquez, E. Lastochkin, B. Boggess, S. Mobashery

103. Design, synthesis, and evaluation of novel inhibitors of OXA-carbenemases. **A.A. Bastian**, N. Stewart , N.T. Antunes , M. Kumarasiri, S. Vakulenko, S. Mobashery*

104. Antibiofilm studies using catheters with controllable electrochemical nitric oxide releas. **H. Ren**, J. Wu, C. Xi, M.E. Meyerhoff

105. Design and synthesis of simplified caramazycin analogs. **T. Nakaya**, A. Matsuda, S. Ichikawa

106. Some novel divalent metal based drug complexes: Preparation, analysis, and biological activities investigations. **J.A. OBALEYE***, N. Simon, B.U. Eke, A.C. Tellis, M.O. Barnigboye, P.F. Omojasola, E.A. Balogun, J.O. Adebayo

107. Hydrogel-based contact active antimicrobial coatings. **M. Chan-Par***

108. Nanoparticle hybrid photosensitizers for broad-spectrum, enhanced photodynamic inactivation of bacteria. **B. Hu, X. Cao, T. Ozkaya Ahmadov, H. Tang, P. Zhang***

109. Pathogen neutralization with ionic liquids to treat persistent skin infections.

R. Del Sesto*, A. Koppisch, D.T. Fox, A. Newsham, M. Jones, T. Kern, K. Merrett, N. Nieto, M. Zakrewsky, S. Mitragotri

Hawaii Convention Center
Halls I, II, III

Drug Conjugates: Approaches to Delivering Active Drugs to Where they are Needed (#385)

Organized by: N. Ihle, B. Denny, S. Roffier

Presiding: N. Ihle

Poster Session

10:00 – 12:00

110. Quest for the appropriate enzymatic activity: Cell-in-a-Box® live-cell encapsulation technology for targeted cannabinoid-based chemotherapy. **R.M. Hyslop**

111. Induction of antitumor effect by recruiting the endogenous IgG through a small cross-linker. **K. Sasaki***, D. Funamoto, A. Kishimura, T. Mori, Y. Katayama

* Principle Author

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onlineprogram

- 112.** Human-derived fusogenic peptides for intracellular delivery of proteins.
K. Sudo*, K. Niikura, K. Fujiwara, N. Doi
- 113.** Potent DNA crosslinking cytotoxins as novel payloads for ADCs. **A. Giddens***, M. Bonnett, H.H. Lee, G. Lu, M. Tercel, W. Denney, J.A. Flygare, T.H. Pillow, B.S. Safina, L.R. Staben, V.A. Verma, B. Wei

Hawaii Convention Center
Halls I, II, III

Spectroscopic Tools for the Treatment of Cancer (#397)

Organized by: N. Miyoshi, B. Wilson, W. Ahn, M. Cherukuri

Poster Session
10:00 – 12:00

- 122.** Photodynamic therapy to biliary duct cancer by using fine multichannel endoscope. **K. Kasuya***, R. Soya, Y. Nagakawa, T. Ito, M. Shimazu, A. Tsuchida
- 123.** Enhancement of photodynamic therapy effects with mitochondrial reactive oxygen species. **H. Ito***, H. Matsui, M. Tamura, T. Kaneko, I. Hyodo, H.P. Indo, H.J. Majima
- 124.** Mechanism of porphyrin metabolism in cancer spheroid after administration of 5-aminolevulinic acid. **T. Nakayama***, K. Matsumoto, T. Tanaka, I. Okura, S. Ogura
- 125.** Photosensitizer effect of 9-hydroxyphenoxyphorphoride a on diode laser-irradiated laryngeal cancer cells: Oxidative stress-directed cell death and migration suppression. **P. He***
- 126.** Effect of electron transport chain on the production of PpIX in hypoxia. **S. Otsuka***, K. Matsumoto, T. Tanaka, I. Okura, S. Ogura
- 127.** Control of photodynamic activity of porphyrin photosensitizers through interaction with DNA. **K. Hirakawa***, S. Okazaki
- 128.** Development of PDT system based on composite-type optical fiberscope. **K. Oka***, T. Seki, J. Usuda, T. Kokubo, S. Minakawa
- 129.** Verification of hydroxyl radical density generated in water by low-LET radiation. **Y. Ogawa***, K. Matsumoto

Royal Hawaiian
Regency II

Spectroscopic Tools for the Treatment of Cancer (#397)

Organized by: N. Miyoshi, B. Wilson, W. Ahn, M. Cherukuri
Presiding: K. Hirakawa, Z. Huang

- 8:00 – 114.** Challenges of multidrug resistance in photodynamic therapy of cancer. **Z. Huang**
- 8:30 – 115.** Contribution of singlet oxygen and electron transfer-mediated mechanisms on the photodynamic effect of phosphorus(V)porphyrin. **K. Hirakawa***
- 9:00 – 116.** Enhanced tumor optical imaging and photodynamic effect through albumin-embedding. **M. Huang***
- 9:25 – 117.** Synthesis and photocytotoxicity of fluorophenylporphyrin derivatives having two different functional groups. **S. Hirohara**, Y. Kubota, N. Akiyama, M. Obata, H. Matsui, K. Kakiuchi
- 9:50 Break**
- 10:00 – 118.** Optical properties of a new water soluble chlorin photosensitizer. **Z. Huang**
- 10:25 – 119.** Organic synthetic approach to novel porphyrinoid photosensitizer. **H. Shimakoshi***, Y. Hisaeda
- 10:50 – 120.** Nitric oxide involves cancer specific hematoporphyrin derivatives accumulation via HCP-1 expression. **M. Terasaki**, H. Ito, H. Matsui*
- 11:15 – 121.** Synthesis and characterization of water-soluble polymers bearing porphyrin moiety at the initiating end for photodynamic therapy. **M. Obata***, Y. Tsutsui, S. Hirohara

Wednesday Afternoon

Sheraton Waikiki
Oahu

Chemistry for Development of Theranostic Radiopharmaceuticals (#11)

Organized by: D. Wilbur, M. Adam, P. Donnelly, Y. Arano, J. Jeong, X. Zhang
Presiding: Y. Arano, P.S. Donnelly

- 13:00 – 130.** Potential problems with using radioiodine in development of astatinate-211 theranostic radiopharmaceuticals. **D. Wilbur***, D. Hamlin, M. Chyan, E.R. Balkin, O. Press, B. Sandmaier

- 13:30 – 131.** Development of astatinate-labeled benzylguanidine derivatives for use in cancer pretargeting. **M.D. Hylarides**, D. Wilbur, D.H. Hamlin, C. Ming-Kuan, S.H. Frost, S.L. Frayo, O.W. Press

- 13:45 – 132.** Development of iodine-131-labeled α -methyl-L-phenylalanine for tumor therapy. **H. Hanaoka***, Y. Ohshima, A. Yamaguchi, Y. Suzuki, T. Uehara, N.S. Ishioka, K. Endo, Y. Arano, Y. Tsushima

- 14:00 – 133.** Retinoid based potential theranostic agents for the treatment of atypical teratoid/rhabdoid tumor. **K.F. Ginn**, B.C. Das

- 14:15 – 134.** Evaluating the $^{123}\text{I}/^{211}\text{At}$ therapeutic pair using octreotate modified with a boron cage moiety. **J.R. Crawford***, F. Benard, K. Lin, H. Yang, I. Dude, C. Ming-Kuan, Z. Zhang, P. Schaffer, D. Wilbur, T. Ruth

- 14:30 – 135.** Synthesis and evaluation of Lu-177 labeled somatostatin analog DOTAPasireotide for tumor imaging. **F. Liu**, H. Zhu, X. Chiyi, C. Li, Z. Yang*
- 14:45 Break**
- 15:00 – 136.** Toward reducing renal radioactivity levels of radiolabeled polypeptides. **Y. Arano***

- 15:30 – 137.** Theranostic application of cancer targeting probes labeled with various copper radioisotopes. **T. Saga***

- 16:00 – 138.** Ga-68 radiopharmaceuticals and their quality control. **P. Roselt***

- 16:30 – 139.** ^{44}Sc : From bench to bedside. **N. van der Meulen***, C. Müller, K. Dominich, M. Bunka, C. Vermeulen, A. Singh, R. Baum, A. Türler, R. Schibli

- 16:45 – 140.** Multifunctional radiolabeled combined peptides for theranostics of primary cancer and bone metastases. **K. Ogawa**, J. Yu, A. Ishizaki, M. Yokokawa, Y. Kitamura, K. Shiba, M. Odani

- Sheraton Waikiki
Waianae

- Fragment-based Lead Discovery (#145)**
- Organized by:* D. Erlanson, M. Scanlon, K. Ruan, D. Tanaka, J. Tyndall
Presiding: J. Tyndall

13:00 Fragments to leads and drugs

- 13:00 – 141.** Fragment-based approach for targeting kinases. **C. Sun***

- 13:30 – 142.** Selective inhibition of BRM bromodomain and chromatin interaction. **K. Ruan***

- 14:00 – 143.** Fragment-based drug discovery of potent and selective CYP121 inhibitors for tuberculosis. **M.E. Kavanagh**, A.G. Coyne, G.G. James, K. McLean, L. Pedro de Carvalho, A.W. Munro, C. Abel

- 14:20 – 144.** Novel McI-1/Bcl-2 dual inhibitors created by the structure-based hybridization of drug-divided building blocks and a fragment deconstructed from a known two-face BH3 mimetic. **Z. Zhang***

- 14:45 – 145.** Fragment library screening identifies hits that bind to the noncatalytic surface of *Pseudomonas aeruginosa* DsbA1. **R.M. Mc Mahon***, K. Rimmer, B. Mohanty, S. Headley, M. Vazirani, M. Coinson, S. Tay, J. Simpson, C. Morton, J. Martin, M. Scanlon

- 15:05 Break**

- 15:15 – 146.** Discovery and characterization of small molecule fragments that bind and inhibit the ubiquitin specific protease 7 (USP7). **P. Di Lello**, T. Crawford, K. Deshayes, J. Drobnick, J. Drummond, J. Ernst, L. Kategaya, C. Ly, T. Maurer, J. Murray, C. Ndubaku, R. Pastor, L. Rouge, V. Tsui, X. Zhao, K. Zobel, I. Wertz

- 15:45 – 147.** Identification of type II inhibitors targeting BRAF V600E using privileged fragment based hybrid-design approach. **Q. Zhang***, F. Wang

- 16:05 – 148.** Selectivity of the initial fragment hits in fragment based drug design approach. **M. Takimoto-Kamimura***

- 16:30 – 149.** FBBL yields orally active, brain penetrant inhibitors for BACE1 and PDE10A. **D.F. Wyss***

Sheraton Waikiki
Waialua

New Antibacterial Agents (#236)

Organized by: J. Finn, J. Palmer, H. Arimoto
Presiding: J. Finn

13:00 Opening Remarks

- 13:05 – 150.** Targeting metallo-beta-lactamases (MBLs) for new antibacterial agents. **M.W. Crowder***, M. Altha, H. Yang, A. Bergstrom, D. Tierney, B. Bennett, L. Sutton, L. Moritz, O. Sanyurah, A. Moller

- 13:30 – 151.** Discovery of new nonantibiotics that restore MRSA susceptibility to β -lactam antibiotics. **H. Tomoda***, N. Koyama

- 13:55 – 152.** Cell wall as target for discovery of novel antibiotics. **S. Mobashery***

- 14:40 – 153.** Disarming antibiotic resistance using an adjunctive strategy. **C. Melander**

- 15:05 break**

- 15:20 – 154.** Synthesis and biological studies of a new class of antibiotic potentialators for methicillin-resistant *Staphylococcus aureus* (MRSA). **E. Speri**, M.A. Boudreau, J. Fishovitz, S. Mobashery*

- 15:45 – 155.** SNAPPING Gram-negative bacteria with star-shaped polypeptides. **S. Lam**, N. O'Brien-Simpson, N. Pantaratt, A. Sulistio, E. Wong, Y. Chen, A. Blencowe, E. Reynolds, G.G. Qiao*

- 16:05 – 156.** Deciphering the structure-activity relationships of tomatidine, a steroid alkaloid with antibiotic properties against small colony variants of *Staphylococcus aureus*. **E. Marsault***, F. Chagnon, I. Guay, M. Lamontagne-Boulet, F. Malouin

- 16:25 closing remarks**

Sheraton Waikiki
Kohala/Kona

Drug Conjugates: Approaches to Delivering Active Drugs to Where they are Needed (#385)

Organized by: N. Ihle, B. Denny, S. Roffler
Presiding: N. Ihle

13:00 Introductory Remarks

- 13:05 – 157.** Design, synthesis, and evaluation of novel anabolic bone-targeting prodrugs for treatment of osteoporosis and other bone conditions. **R.N. Young***, G. Chen, H. Xie

- 13:45 – 158.** Development of antibody drug conjugates for cancer therapy. **P. Senter**

- 14:25 – 159.** Novel chemistries for antibody-drug conjugates. **T. Pillow**

- 15:05 BREAK**

- 15:20 – 160.** pH-tunable linker: The next generation of versatile linkers for ADC. **C.J. Choy**, C. Berkman

- 15:40 – 161.** New molecular transporters and nanovaults for drug/probe delivery: Targeting resistant disease and AIDS eradication. **P.A. Wender***

- 16:20 – 162.** Self-assembling drug conjugates. **H. Cui**

Royal Hawaiian
Regency II

Spectroscopic Tools for the Treatment of Cancer (#397)

Organized by: N. Miyoshi, B. Wilson, W. Ahn, M. Cherukuri
Presiding: H. Matsui, T. Yamamoto

- 13:00 – 163.** Cancer cellular treatments with heavy atoms involved fluorescent X-ray. **H. Matsui***, H. Ito, M. Terasaki, M. Tamura, T. KANEKO

- 13:20 – 164.** Boron neutron capture therapy for glioblastoma. **T. Yamamoto***, K. Nakai, H. Kumada, T. Aihara, E. Sato, T. Isobe, A. Matsumura

- 13:40 – 165.** Carbon-ion therapy for patients with liver, pancreatic, and colorectal cancer. **S. Yamada***, N. Okada, S. Yasuda, Y. Isozaki, T. Kamada

- 13:55 – 166.** Reactive oxygen species induced by X-ray and heavy-ion beam. **K. Matsumoto***, Y. Ogawa, M. Ueno, I. Nakanishi

- 14:10 – 167.** Stereotactic body radiation therapy for non-small cell lung cancer, and hepatocellular carcinoma: Japanese experience. **T. Kimura**

- 14:25 – 168.** Development of the accelerator based neutron source for BNCT in University of Tsukuba. **H. Kumada**, A. Matsumura, H. Sakurai, M. Yoshioka, H. Kobayashi, H. Matsumoto, T. Kurihara, T. Nakamura, H. Nakashima, T. Sugano, N. Ikeda

- 14:40 – 169.** Development of new boron delivery system for BNCT clinical trial. **K. Nakai**, T. Yamamoto, H. Kumada, A. Aihara, F. Yoshida, A. Matsumura

14:55 Break

- 15:05 – 170.** On-time imaging of the distribution of ^{10}B in BNCT by the detection of 478keV prompt gammas with Electron Tracking Compton Camera. **T. Tanimori***

- 15:20 – 171.** ROS generation and radiosensitization by gold nanoparticles under MV X-ray irradiation. **M. Misawa***, M. Hayano, M. Sato, J. Takahashi, K. Fujita, K. Hayashi

- 15:35 – 172.** Boron-neutron capture therapy for head and neck cancer. **T. Aihara**, H. Ishikawa, H. Kumada, N. Fukumitsu, K. Ohnishi, J. Hiratsuka, T. Yamamoto, A. Matsumura, H. Sakurai

- 15:50 – 173.** Non-platinum-based halogenated compounds: A new class of potent anti-tumor agents in combination with radiation therapy. **Q. Lu***, C. Wang, Q. Zhang, Y. Wu, Y. Mei, J. Warrington, N. Ou

Wednesday Evening

Sheraton Waikiki
Waianae

Fragment-based Lead Discovery (#145)

Organized by: D. Erlanson, M. Scanlon, K. Ruan, D. Tanaka, J. Tyndall
Presiding: D. Erlanson

19:00 Poster popcorn

19:20 Special topics: TBA

19:40 Practical FBLD discussion

* Principle Author

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Sheraton Waikiki
Oahu

Spectroscopic Tools for the Treatment of Cancer (#397)

Organized by: N. Miyoshi, B. Wilson, W. Ahn, M. Cherukuri

19:00 – 174. Review of Session-I-III includes Posters (PDT/Clinics and Photosensitizers). **W. Ahn**

19:15 – 175. Review of Sessions-I-III includes Posters (PDT, SDT /Veterinary Animals). **Y. Okamoto**

19:30 – 176. Review of Session-II (FT-IR, Raman/Clinical screening and tumor model). **N. Miyoshi**

19:45 – 177. Review of Session-II (Terahertz/Imaging and Hyperthermia). **Y. Ogawa**

20:00 – 178. Review of Session-III. -I includes Posters (PDT/Photosensitizers, Mechanisms). **Z. Huang**

20:15 – 179. Review of Session-III. -I includes Posters (PDT/Photochemistry, Active oxygen species). **K. Hirakawa**

20:30 – 180. Review of Session-IV includes Posters (Fluorescent X-ray/Cells and Animals). **H. Matsui**

20:45 – 181. Review of Session-IV includes Posters (BNCT, Proton, Carbon / Clinics and Animals). **T. Yamamoto**

Thursday Morning

Hawaii Convention Center
Halls I, II, III

Oligonucleotide Therapeutics: From Base Pairs to Bedsides (#8)

Organized by: M. Manoharan, M. Damha, T. Wada

Presiding: V. Mohan

Poster Session **10:00 – 12:00**

182. Discovery of a “DNA zip-slider” domain in human RecQL helicases WRN and BLM. **K. Kitano***, S. Kim, T. Hakoshima

183. Intracellular delivery analysis of siRNA therapeutics based on siRNA-selective fluorescent probes. **Y. Sato**, T. Sato, M. Kaneko, S. Nishizawa*

184. Synthesis and properties of oligonucleotides containing P3'->S5' phosphorothioates. **A. Fujisaka***, M. Islam, R. Waki, K.R. Ito, S. Obika

185. Synthesis of saccharide-modified oligonucleotide as an inhibitor of influenza virus infection. **Y. Nomura**, M. Matsuda, M. Yamabe, D. Akamatsu, Y. Ebara*

186. Synthesis of mannose-modified oligonucleotide that bind to mannose binding protein. **M. Matsuda**, Y. Nomura, M. Yamabe, D. Akamatsu, Y. Ebara*

187. Synthesis and properties of P-stereodefined PO/PS-chimeric oligoribonucleotides. **Y. Nakaga**, N. Oka, T. Wada*

188. Use of 4-nitrobenzyl group for the development of therapeutic oligonucleotides. **Y. Hiyoshi**, K. Iketani, K. Kondo, A. Ono, H. Saneyoshi

189. Creation of the hypoxia-specific oligonucleotide therapeutics system with intracellular environment-responsive peptide ribonucleic acids (PRNs): Synthesis and antisense activities of new type of chimeric PRNA-DNA derivatives containing phosphoramidate linkage in PRNA-DNA junction. **M. Inagaki**, R. Uematsu, Y. Araki, S. SAKAMOTO, s. ishibashi, H. Kashida, H. Asanuma, T. Yokota, T. Wada*

190. Reduction-activatable protecting groups for pro-oligonucleotides. **K. Kondo**, K. Iketani, A. Ono, H. Saneyoshi

191. Creation of hypoxia specific oligonucleotide therapeutics system with intracellular environment-responsive peptide ribonucleic acids (PRNs): Tuning and optimization of on – off switching pH of PRNA for hypoxia specificity. **M. Asai**, R. Uematsu, Y. Araki, S. SAKAMOTO, s. ishibashi, T. Yokota, T. Wada*

192. Remarkable cellular uptake enhancement of arginine introduced peptide ribonucleic acid (PRNA) for hypoxia specific oligonucleotide therapeutics. **H. Sugai**, I. Nakase, S. SAKAMOTO, Y. Araki, M. Takai, T. Wada

Sheraton Waikiki
Oahu

Chemistry for Development of Theranostic Radiopharmaceuticals (#11)

Organized by: D. Wilbur, M. Adam, P. Donnelly, Y. Arano, J. Jeong, X. Zhang

Presiding: J. Jeong, X. Zhang

8:00 – 193. Beginnings, evolution, and current status of “theranostics”. **S.C. Srivastava***

8:30 – 194. Novel treatments for arthritis in humans and animals using the theranostic isotope Sr-117m: Colloids and labeled molecules. **N.R. Stevenson***, J. Simon

8:45 – 195. Intrinsically radioactive nanoparticles for tumor imaging. **X. Chen***

9:15 – 196. Folate-conjugated polymers with ^{99m}Tc for tumor imaging. **Z. Guo**, P. Zhang, M. Song, R. Zhuang, C. Liu, X. Zhang*

9:45 – 197. Radiopharmaceutical evaluation of peptide nucleic acid bi conjugates as complementary system for tumor pretargeting. **H. Stephan**

10:00 Break

10:15 – 198. Development of multifunctional nanoparticles by encapsulation with special amphiphiles. **J. Jeong***

10:45 – 199. Development of PSMA targeting therapy using Lu-177-labeled nanoparticles. **S. Oh**, S. Moon, J. Jeong*, D. Lee

11:15 – 200. Lanthanide upconversion nanoparticles for biomaging. **F. Li***

11:45 – 201. Dragon fruit-like biocage as an iron trapping nanoparticle for high efficiency targeted cancer multimodality imaging. **M. Yang***, Q. Fan, R. Zhang, K. Cheng, J. Yan, D. Pan, Z. Cheng

Sheraton Waikiki
Waianae

Advances in Polymers for Medicine (#52)

Organized by: J. Pokorski, R. Advincula, T. Miyata, C. Boyer, K. Ishihara, Presiding: J. Pokorski

8:00 – 202. Dense peptide brush polymers as delivery systems for therapeutic peptides. **N. Gianneschi**

8:30 – 203. Shaping plant virus-based nanoparticles for applications in biomedical imaging and therapeutic intervention. **N.F. Steinmetz***

9:00 – 204. Drug-free macromolecular therapeutics - a new paradigm in polymeric nanomedicines. **J.H. Kopecek***, T. Chu, J. Yang, R. Zhang, J. Hartley

9:30 Coffee Break

9:50 – 205. Breakthroughs in imprint lithography and 3D additive fabrication to advance NextGen drug delivery technologies. **J.M. DeSimone***, **J.C. Lufft**

10:20 – 206. Molecularly imprinted nanogel particles that acquire stealth in situ by cloaking themselves with the body's own dysposonic protein. **T. Takeuchi***, R. Sasa, Y. Kitayama

10:40 – 207. Molecular imaging MRI agents responsive to biological signals. **C. Zhang, K. Wang, H. Peng, s. puttick, K. Thurecht, S. Rose, A. Whittaker**

11:10 – 208. Polymer-based nanoparticles cancer therapeutics: From concept to clinic. **M.E. Davis**

Hawaii Convention Center
Halls I, II, III

Fragment-based Lead Discovery (#145)

Organized by: D. Erlanson, M. Scanlon, K. Ruan, D. Tanaka, J. Tyndall

Poster Session

10:00 – 12:00

209. Novel tools for screening fluorine containing fragments by NMR. **C. Ankin**, H. Kovacs

210. Redesign of the Merck Fragment Library. **C. Fischer***

211. Identification of novel activators of casinolytic protease p using fragment based screening approaches. **A.P. Singh***, Y. Zhao, Z. Zheng, E. Griffith, W. Shadrick, R. Tangallapally, J. Bowling, **R. Lee***

212. Similarity analyses of ligand-binding subsites on proteins. **N. Yamaotsu***, S. Hiroto

213. Natural products = Frequent hitters?. **P. Schneider***

Hawaii Convention Center
Halls I, II, III

Chemistry of Molecular Imaging (#215)

Organized by: H. VanBrocklin, G. Tamagnan, Y. Fujibayashi, L. Luyt, A. Katsifis, Y. Choe, N. Vasdev

Presiding: H. VanBrocklin, D. Wilbur

Poster Session

10:00 – 12:00

214. ¹¹C-labeling of the C(1)–C(10) dihydroxy acid moiety for the study on the synthesis of kurokekahilide-2 PET tracer. **C. Han***, H. Doi, J. Kimura, Y. Nakao, M. Suzuki*

215. ¹⁸F-labeled FSHR antagonist for PET imaging of prostate cancer. **D. Pan**, Y. Xu, J. Yan, R. Yang, L. Wang, M. Yang*

216. New theranostic probe for tumor hypoxia based on triple-resonance NMR and radio-sensitization. **Y. Suzuki**, H. Yamada, Y. Kimura, A. Son, K. Tanabe, A. Toshimitsu, Y. Aoyama, T. Kondo*

217. Biocompatible phosphorylcholine polymer probes for *in vivo* photoacoustic imaging. **N. Matsumoto**, H. Yamada, Y. Kimura, A. Toshimitsu, Y. Aoyama, T. Kondo*

218. Catabolism of a ⁶⁴Cu- and Cy5.5-labeled human serum albumin in a tumor xenograft model. **C. Kang**, H. Koo, G. An, Y. Choe*

219. Densely iodinated stealth dendrimers as blood-pool contrast agents for computed tomography. **Y. Kim***, H. Jung, S. You

220. Dual imaging agent for ultrasound and PET: Nanodroplets encapsulated perfluorocarbon and [Cu-64]ATSM. **K. Lee**, U. Shin, J. Lee, H. Park, G. An, C. Choi, S. Lim, B. Kim, J. Seo, J. Kim

221. Electrochemical radiofluorination of sulfur containing aliphatic acids: Potential approach to radiolabeling of amino acids. **A. Lebedev***, Q. He, F. Yang, S. Sadeghi

222. Electrochemical radiolabeling of COX-2 inhibitors: Potential PET agents for imaging of inflammation. **A. Lebedev***, Q. He, S. Sadeghi

223. Evaluation of simultaneous dual-isotope SPECT/PET/CT imaging with ^{99m}Tc and ⁶⁴Cu by phantom study and its *in vivo* application. **N. Adachi***, Y. Yoshii, T. Furukawa, Y. Takeuchi, M. Inubushi, H. Wakizaka, M. Zhang, Y. Fujibayashi, T. Saga

224. Hyperpolarized ¹⁵N tripodal tetramine derivatives as sensors of free Zn²⁺ ions *in vivo*. **E. Suh***, L. Limata, A. Sherry, Z. Kovacs

225. Evaluation of TiOH base for Pd⁰-mediated coupling of methyl iodide and excess boronic acid esters toward fabrication of short-lived ¹¹C-incorporated PET tracer. **H. Koyama**, H. Doi, M. Suzuki*

226. Hyperpolarized NMR molecular probe for long-term biomolecule analysis. **M. Hirano***, H. Nonaka, S. Sando

227. Rh(I)-mediated rapid ^{[14}C]carboxylation using ^{[14}C]CO₂ and organoborane at atmospheric pressure. **M. Goto**, S. Kurai, R. Yamamoto, T. Kanamitsu, M. Suzuki, Y. Watanabe, H. Doi*

228. Probe-targeted magnetic resonance imaging of tumor with a self-traceable ¹H-¹³C polymeric nanoprobe. **H. Yamada***, Y. Hasegawa, Y. Kimura, H. Imai, T. Matsuda, Y. Uto, Y. Aoyama, T. Kondo

229. Non-invasive PET imaging of the glucagon-like peptide-1 receptor in the pancreas with ¹⁸F labeled exendin-4 analog. **Y. Xu**, D. Pan, R. Yang, L. Wang, J. Yan, M. Yang*

230. Micelle type dual imaging probe for positron and near-infrared fluorescence imagings. **A. Makino**, A. Tomoike, H. Kimura, M. Ono, H. Okazawa, Y. Kiyono, H. Saji

231. Binding of indium, gallium, and ruthenium ions by gastrins for biomedical applications. **J.M. Pushie**, G.N. George, G.S. Baldwin

232. Impact of chelating agent on MMP-binding. **S.C. Ghosh**, N. Wilgowski, E.M. Sevick-Muraca, A. Azhdarina*

233. Development of 2-[¹¹At]astatato- α -methyl-L-phenylalanine (2-AAMP) as a novel radiopharmaceutical for internal radiotherapy. **Y. Ohshima***, H. Suzuki, H. Hanaoka, S. Watanabe, S. Watanabe, N. Watanabe, Y. Tsushima, K. Endo, Y. Arano, N.S. Ishioka

234. In-situ preparation of trivalent ^{99m}Tc/^{186/188}Re-labeled compounds from monovalent ligand for ready-to-use theranostic radiopharmaceuticals: Factors affecting radiochemical yields of isonitrile-based trivalent ^{99m}Tc/^{186/188}Re-labeled compounds. **Y. Mizuno**, C. Jen, T. Uehara, Y. Arano

235. Synthesis and biological evaluation of a ^{99m}Tc-labeled fatty acid for myocardial metabolic imaging. **L. Jianping**, x. qianqian, Z. huabei*

236. Synthesis and biological evaluation of novel ⁶⁴Cu-labeled dimeric c(RGD-ACH-K) peptide conjugates for tumor PET imaging. **K. Lee***, J. Park, J. Lee, U. Shin, G. An, J. Kim*

237. Synthesis of ⁸⁹Zr-labeled trastuzumab and thio-trastuzumab for PET imaging of HER-2 positive lesions. **K. Lee**, J. Lee, U. Shin, J. Park, H. Park, G. An, C. Choi, S. Lim, B. Kim, J. Kim

238. Synthesis and evaluation of a N-13 labeled nitric oxide donor, 3-methyl-4-fuoroxan carbalddehyde for preliminary PET imaging. **A.B. Pippin***, R.J. Voll, M. Smith, D.C. Liotta, M.M. Goodman

239. Toward convenient synthesis of ¹⁸F-labeled MIBG analogs. **A. Yamaguchi**, H. Hanaoka, T. Higuchi, Y. Tsushima

240. Tropomyosin receptor kinase (TrkA/B/C) PET imaging: Synthesis and structure – activity relationship studies of fluorinated (2-(3-fluorophenyl)pyrrolidin-1-yl)imidazo[1,2-b]pyridazine-based inhibitors. **V. Bernard-Gauthier**, R. Schirrmacher

Sheraton Waikiki
Honolulu

New Antibacterial Agents (#236)

Organized by: J. Finn, J. Palmer, H. Arimoto

8:00 Opening remarks

*** Principle Author**

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8:05 – 241. Targeting HSP60/10 (GroEL/ES) chaperonin systems as a mechanistically unique antibiotic strategy. S.J. Abdeen, N. Salim, R. Veeramachaneni, A. Ambrose, P.G. Schultz, A. Horwitz, E. Chapman, **S.M. Johnson***

8:30 – 242. Discovery and optimisation of new small-molecule inhibitors of bacterial DNA gyrase and topoisomerase IV.

N. Stokes*

9:00 – 243. VXc-486, a novel dual targeting GyrB/ParE inhibitor for the treatment of bacterial infections: Discovery and characterization of a water-soluble prodrug. **H. O'Dowd**

9:30 – 244. CRS3123, a novel diaryldiamine in clinical development for treatment of *Clostridium difficile* infection. **T. Jarvis***, S. Bell, I. Critchley, D. Davies, D. Drolet, S. Gill, J. Guiles, U. Ochsner, J. Rohloff, X. Sun, N. Janjic

10:00 break

10:15 – 245. SBDD approach of the novel inhibitor of bacterial multidrug efflux transporter. **Y. Inoue***, S. Yamasaki, Y. Higuchi, A. Yamaguchi, N. Kato

10:40 – 246. Targeting *nusB-nusE* binding to inhibit antitermination, a novel antibiotic target. **P. Cossar***, C. Ma, J.I. Ambrus, P.J. Lewis, A. McCluskey

11:05 closing remarks

Sheraton Waikiki
Waialua

Nutraceuticals and Functional Food Ingredients: Chemistry and Health (#285)

Organized by: F. Shahidi, C. Ho, R. Pegg, K. Miyashita
Presiding: C. Ho, K. MIYASHITA, F. Shahidi

8:00 opening

8:05 – 247. Novel phenolic antioxidants: performance and role in health and disease. **F. Shahidi***

8:25 – 248. Bioavailable antioxidants to suppress the formation of 8-hydroxy-2'-deoxyguanosine in oxidative injury of DNA. **K. Kanazawa***, K. Kanazawa

8:45 – 249. Vitamins potently inhibit thiyl radical-induced *trans* fatty acid formation in PC-12 cells. **W. Hung**, C. Ho, L.S. Hwang

9:05 – 250. Flaxseed dietary fibre association with phenolic compounds and their bioactivity. **F. Hosseiniyan***

9:25 – 251. Relationship between in vitro and biological antioxidant assay of pecan phenolics. **R.B. Pegg***, M. Kellett, Y. Gong, P. Greenspan

9:45 break

9:55 – 252. Controlling the gastrointestinal fate of nutraceutical-enriched lipid delivery systems for improved bioavailability. **H. Xiao***

10:15 – 253. A multiple bioactivity of flavan-3-ols was revealed through sympathetic nerve stimulation. **N. Osakabe***, N. Kami, K. Inagawa

10:35 – 254. Dietary factors affecting bioavailability of onion flavonoids. **J. Terao***

10:55 – 255. Bioactive properties of orange peel on intestinal antioxidant, anti-inflammatory activities and cell tight junction function. **X. Chen***, D. Kitts

11:15 – 256. Antioxidant and cytoprotective activities of solventless extracts from fruit and vegetable wastes. **M.Y. Heng**, S. Katayama, E. Ong, S. Nakamura

11:35 – 257. Compounds isolated from *Osmanthus fragrans* var. *thunbergii* and their properties of antioxidant and anti-proliferative. **B. Lu**, F. Zhou

11:55 closing

Sheraton Waikiki
Kohala/Kona

Drug Conjugates: Approaches to Delivering Active Drugs to Where they are Needed (#385)

Organized by: N. Ihle, B. Denny, S. Roffler
Presiding: M. Tercel

8:00 Introductory Remarks

8:05 – 258. Arming antibodies with DNA cross-linking agents derived from the duocarmycins. **M. Tercel***, A. Giddens, G. Lu, H.H. Lee, M. Bonnet, W. Denny, J.A. Flygare, T.H. Pillow, B.S. Safina, L.R. Staben, V.A. Verma, B. Wei

8:45 – 259. Development of novel diketoperazine-forming spacer: Gly-Pro. **S. Manabe***, Y. Aihara, H. Machida, M. Yasunaga, Y. Ito, Y. Matsumura

9:05 – 260. Optimization and tumor targeting of 1,2-bis(sulfonyl)hydrazines.

P.G. Penketh*, K. Shyam, R. Baumann, K. Ishiguro, R. Zhu, A. Sartorelli

9:45 BREAK

10:00 – 261. α -Galactosidase A loaded nanoliposomes with enhanced enzymatic activity for Fabry disease. **J. Veciana***, I. Cabrera Puig, I. Abasolo, J. Corchero, E. Elizondo, P. Rivera, E. Moreno, J. Faraldo, S. Salas, M. Bueno, M. Rivas, M. Melagarejo, D. Pulido, M. Royo, F. Albericio, A. Villaverde, M. Parajo, S. Schwartz, N. Ventosa

10:20 – 262. Discovery of TH-4000: A renaissance in hypoxia-activated prodrug design. **J. Small***, G. Lu, H.H. Lee, S. Silva, V. Jackson, M. Abbattista, C. Guise, M. Bull, A. Grey, H. Hsu, J. Sun, J. Jaiswal, S. Jamieson, A. Ashoorzadeh, R. Anderson, C. Hart, T. Pearce, A. Patterson

11:00 – 263. Therapeutic targeting of the hypoxic compartment of the tumor microenvironment with evofosfamide (TH-302): Translational and clinical studies. **M. Matteucci**

Thursday Afternoon

Sheraton Waikiki
Waianae

Advances in Polymers for Medicine (#52)

Organized by: J. Pokorski, R. Advincula, T. Miyata, C. Boyer, K. Ishihara
Presiding: T. Miyata

13:00 – 264. Catalysis of endogenous therapeutics at medical polymer interfaces – an alternative approach for long term device integration. **M. Reynolds***, M. Neufeld, E. Lauzon, A. Lutzke, A. Pegalajar-Jurado

13:20 – 265. Delivery of carbon monoxide using polymeric nanoparticles for bioapplications. **C. Boyer**, D. Nguyen, K. Nguyen

13:40 – 266. Biomaterials processed via melt extrusion: Molecular modification of scalable nanofibers. **J. Pokorski**

14:00 – 267. Thermally-driven self-cleaning membranes: Extending the lifetime of an implanted glucose biosensor. **M.A. Grunlan***

14:20 – 268. Directing cellular functions via hydrated mobility of polyrotaxane surfaces. **N. Yu***, J. Seo, T. Yamaoka, S. Kakinoki

14:50 Break

15:00 – 269. Photoinduced and self-initiated graft polymerization of 2-methacryloyloxyethyl phosphorylcholine on poly(ether ether ketone) for obtaining surface biocompatibility. **K. Ishihara***

15:30 – 270. Engineering biointerfaces using controlled radical polymerization. **H. Klok**

15:50 – 271. Graphene oxide/polymer antimicrobial agents and polymeric coatings. **R. Advincula***

16:10 – 272. Fabrication of drug crystalline-loaded polymer thin films (nanosheets) for biomedical applications. **S. Takeoka***, K. Ito, K. Nishiwaki, T. Fujie

16:30 – 273. Rapid neointima formation and good patency of very thin long bypass grafts with circulating cell-capturing surface. **T. Yamaoka***, M. Kitai, A. Otaka, M. Munisso, Y. Ohya, A. Mahara

Sheraton Waikiki
Oahu

Chemistry of Molecular Imaging (#215)

Organized by: H. VanBrocklin, G. Tamagnan, Y. Fujibayashi, L. Luyt, A. Katsifis, Y. Choe, N. Vasdev
Presiding: G. Tamagnan, H. VanBrocklin

13:00 Opening Remarks

13:10 – 274. Low temperature nucleophilic F-18 fluorination for bioconjugation chemistry. **D. Chi***, B. Lee, B. Kang

13:45 – 275. Iodonium ylide mediated radio-fluorination: A general method for the preparation of PET radiopharmaceuticals. **S. Liang***, N. Vasdev

14:05 – 276. Copper-mediated approaches to late-stage fluorination with fluorine-18. **A. Brooks**, N. Ichishi, A. Mossine, K. Makaravage, J. Miller, J. Topczewski, M. Sanford, **P.J. Scott**

14:25 – 277. Discovery and optimization of tracer ligands for CNS PET imaging. **S. Hitchcock***

15:00 Break

15:20 – 278. Imaging platform sensitive to protease activity for detection of Alzheimer's disease. **J. Snir**, M. Suchy, G.A. Bindsell, R. Ta, K. St. Lawrence, **R. Hudson***, S. Pasternak*, R. Barth*

15:40 – 279. Fluorine-18 labeled PET imaging tracer targeting the astroglial CNS excitatory amino acid transporter 2 protein. **J.E. Blecha**, S. Ahmed, J. Gerdes, H. VanBrocklin

16:00 – 280. Transport of $[^{11}\text{C}]$ vitamin C and redox partner $[^{11}\text{C}]$ dehydroascorbic acid in human glioma cells. **V.N. Carroll**, C. Truillet, B. Shen, X. Shao, P. Scott, F. Chin, D. Wilson

16:20 – 281. D- and L- [$[^{18}\text{F}]$]-fluoro amino-suberic acid ($[^{18}\text{F}]$ -FASU) for oxidative stress imaging. **H. Yang**, S. Jenni, Q. Miao, I. Rodrigo, C. Poleschuk, J.M. Webster, F. Benard, P. Schaffer

16:40 – 282. Redox-responsive MRI contrast agents. **E. New***, E. O'Neill, K. Jankowska, P. Bonnitcha

Sheraton Waikiki
Honolulu

New Antibacterial Agents (#236)

Organized by: J. Finn, J. Palmer, H. Arimoto
Presiding: H. Arimoto

13:00 opening remarks

13:05 – 283. Bringing the full power of chemical synthesis to bear on the discovery of new antibiotics. **A.G. Myers***

13:55 – 284. Multifunctional amphiphilic aminoglycoside antibiotics and adjuvants. **F. Schweizer***, B. Gorityala, G. Guchhait

14:20 – 285. Rational design of antibiotics and NSAIDs. **M.A. Cooper**

14:45 Break

15:00 – 286. Van-M-5427, a novel semi-synthetic glycopeptide with reduced nephrotoxicity. **O. Yoshida**

15:25 – 287. Mechanism of action and epitopes of clostridium difficile toxin B neutralizing antibody bezlotoxumab. **C. Strickland**, P. Orth, L. Xiao, A. Therien, L. Hernandez

15:50 – 288. Antibody-antibiotic conjugates (AACs): A novel therapeutic platform to treat invasive *S. aureus* infections. **T. Pillow**

16:15 – 289. New classes of antitubercular compounds derived from phenotypic screens and developed with different models. **J. Baget**, G. Nagalingam, J. Triccas, P. Rutledge, J. Castro-Pichel, **M. Todd***

16:40 closing remarks

Sheraton Waikiki
Waialua

Nutraceuticals and Functional Food Ingredients: Chemistry and Health (#285)

Organized by: F. Shahidi, C. Ho, R. Pegg, K. Miyashita
Presiding: C. Ho, R.B. Pegg, F. Shahidi

13:00 opening

13:05 – 290. Functional foods for heart health: Managing trimethylamine oxide level through gut microbiota. **C. Ho***, L. Sheen

13:25 – 291. Prevention of procyanidins and cyanidin-3-glucoside on B(a)P-induced DNA damage through modulating drug-metabolizing enzymes hepatocytes. **H. Ashida***, Y. Yamashita, T. Zhang

13:45 – 292. Modulation of neuroprotective genes by natural dietary bioactive compounds in senescence-accelerated mice. **S. Katayama**, S. Nakamura

14:05 – 293. Antiaging effect - from discovery to clinical trial. **C. Wang***

14:25 – 294. Possibility of dietary factors to prevent and treat diabetes via the stimulation of GLP-1 secretion. **T. Tsuda***

14:45 – 295. Safety and efficacy of a novel *Trigonella foenum-graecum* seed (fenugreek seed) extract (Furocyst) in polycystic ovary syndrome in female volunteers. **D. Bagchi***

15:05 break

15:15 – 296. Processing of GABA enriched salt-free soybean paste and its blood pressure lowering effect in human volunteer test. **H. Hatta***, S. Shou, Y. Ueno

15:35 – 297. Adenine, a vasorelaxant, reduces intestinal inflammation in colitis mouse mode. **T. Fukuda**, T. Matsui, Y. Mine*

15:55 – 298. Beyond antioxidant and anti-inflammatory activities of phytochemicals inhibit osteoclastogenesis. **M. Uehara***, H. Inoue, N. Takahashi

16:15 – 299. Dynamic modulation of Nrf2/Keap1 system by nutraceuticals. **D. Hou***

16:35 closing

Thursday Evening

Hawaii Convention Center
Halls I, II, III

Advances in Polymers for Medicine (#52)

Organized by: J. Pokorski, R. Advincula, T. Miyata, C. Boyer, K. Ishihara

Poster Session

19:00 – 21:00

300. Enzymatically functionalized chitosan microspheres for iron sequestration. **D. Huber, A. Pelis, I. Brzozova, G.S. Nyahongo, G.M. Guebitz***

301. Synthesis, characterization, and in vivo evaluation of radiolabeled anti-inflammatory dendritic polyglycerol: A structure – pharmacokinetics relationship. **K. Pant***, D. Gröger, R. Bergmann, J. Pietzsch, H. Stephan, R. Haag

302. Use of biocompatible hydrogel beads for the recovery and delivery of antibiotics. **K. Ko**

303. Glyco-nanoparticles for the delivery of platinum chemotherapeutics. **M. Callari***, J. Aldrich-Wright, P. De Souza, M. Stenzel

* Principle Author

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<http://pacificchem.org/onlineprogram>

- 304.** Amylose-based glyco star polymers: A biofunctional platform for glyco-biomaterials. **T. Nishimura**, S. Mukai, S. Sawada, K. Akiyoshi*
- 305.** Development of pH-sensitive liposomes using hyaluronic acid derivatives for target-specific intracellular drug delivery. **M. Miyazaki**, E. Yuba, H. Hayashi, A. Harada, K. Kono*
- 306.** pH-Sensitive polymer-modified liposomes combined with multiple adjuvants as potent vaccine carriers for cancer immunotherapy. **Y. Yoshizaki**, E. Yuba, N. Sakuchi, K. Koizumi, A. Harada, K. Kono*
- 307.** TiO₂ nanoparticles-incorporated poly-ion complex micelles for effective sono-dynamic therapy. **S. Yamamoto**, E. Yuba, A. Harada, K. Kono*
- 308.** NanoClik microsphere and drug delivery system. **Y. Tahara**, S. Mukai, S. Sawada, Y. Sasaki, K. Akiyoshi*
- 309.** Heparin-mimicking supermolecules for enhancing osteoinduction of bone morphogenetic protein-2. **M. Terauchi**, T. Inada, T. Kanemaru, K. Nishida, A. Tamura, S. Yamaguchi, K. Harada*, N. Yui*
- 310.** Biodegradable three-layered micelles and their hydrogel system as efficient gene delivery vectors. **D.G. Abebe**, R. Kandil, T. Kraus, M. Elsayed, M. Mohammadi, Y. Li, O. Merkel*, T. Fujii*
- 311.** Preparation of photo-responsive polymer particles that form interparticle bondings by UV irradiation and their responsive assembly. **T. Moriyama**, A. Kawamura, T. Miyata*
- 312.** Preparation of self-assemblies from amphiphilic liquid crystalline polymers exhibiting phase transition at body temperature and their drug release behavior. **Y. Inoue**, A. Kawamura, T. Miyata*
- 313.** Fabrication of highly elastic biodegradable hydrogels by dynamic ion-crosslinking with bisphosphonate groups. **M. Noguchi***, A. Nishiguchi, M. Matsusaki, M. Akashi*
- 314.** Controlled drug release from molecularly imprinted polypeptide hydrogels by structural transition of their network. **K. Matsumoto**, A. Kawamura, T. Miyata
- 315.** Two release-rates from carboxymethyl starch monolithic tablets: Formulation, characterization, and in vitro/in vivo evaluation. **C.T. Le***, M. Arella, M. Mateescu
- 316.** Polymer device based on UV-cured poly(ethylene glycol) dimethacrylates for controlled intraocular drug delivery. **N. Nagai***, Y. Izumida, R. Motoyama, E. Koyanagi, A. Katsuyama, S. Yamada, H. Kaji, M. Nishizawa, T. Abe
- 317.** Design of mechanically patterned hydrogel for directing organ bud self-formation. **Y. Shimokawa***, H. Koike, T. Matsuzaki, M. Enomura, M. Kimura, S. Nakabayashi, H. Nakauchi, H. Taniguchi, T. Takebe, H. Yoshikawa
- 318.** Mechanical manipulation of adherent cells by photodegradable hydrogel. **K. Iketaki***, F. Yanagawa, R. Kawamura, S. Nakabayashi, T. Takagi, S. Suguri, T. Kanamori, H. Yoshikawa
- 319.** Chymotrypsin precipitate effects on cell behaviors on silk fibroin. **Y. Tamada***
- 320.** High resisting ability of platelet and NIH3T3 cells adhesion on poly(tetrafluoroethylene-co-vinyl alcohol) coating. **M. Totani**, T. Ando, M. Tanihara, H. Mouri, Y. Tanaka, T. Kanbara, J. Miki
- 321.** Surface modification of PEEK with versatile phospholipid polymer networks. **Y. Kawasaki**, Y. Iwasaki*
- 322.** Antifouling surface modifications of co-extruded polycaprolactone fibers. **A. Advincula**, S. Kim, E. Harker, J. Pokorski
- 323.** Using trichlorosilane surface chemistry to capture endothelial cells: A new approach to overcome restenosis in patients with cardiac stent implants. **R. Ravindranath**, A. Romaschin, M. Thompson
- 324.** Fundamental and applied studies of a novel nitric oxide (NO) releasing polymer-crystal composite with enhanced stability. **Y. Wo***, Z. Li, E.J. Brisbois, A. Colletta, J. Wu, T. Major, R. Bartlett, C. Xi, A.J. Matzger, M.E. Meyerhoff*
- 325.** Surface patterning properties of photo-responsive polymer films and cell culture on their surface. **T. Noguchi**, A. Kawamura, T. Miyata*
- 326.** Glucose-induced decomposition of multilayer film under physiological conditions. **K. Sato***, E. Abe, J. ANZAI
- 327.** Electrochemically controlled release of polymer from 6-ferrocenylhexanethiol monolayer modified electrode. **S. TAKAHASHI***, S. SHIMIZU, J. ANZAI
- 328.** Improved sensing of heparin in whole blood using heparin-imprinted polymer by surface modification or washing. **Y. YOSHIMI***, R. Inaba, T. Ogawa, M. Kanda, M. Inoue, K. Kuwana
- Friday Morning**
- Sheraton Waikiki
Lanai
- De Novo Drug Design (#28)**
- Organized by: G. Schneider, D. Winkler, K. Funatsu, Y. Okuno
Presiding: K. Funatsu, G. Schneider
- 8:00** Opening Remarks
- 8:05 – 329.** Recent progress in structure-based de novo design. **H. Boehm**
- 8:45 – 330.** De-novo design, polypharmacology and metabolism in the generation of novel lead candidates. **R.C. Glen***, M. Wang
- 9:15 – 331.** Site-Hopper: A unique method for binding site comparison. **G.L. Warren**, M. Geballe, T. Darden, J.M. Word, R. Tolbert
- 9:45** Break
- 10:05 – 332.** Computer-aided drug design assisted by synthetic accessibility prediction and target/off-target prediction. **Y. Fukunishi**
- 10:45 – 333.** Prediction of compound-protein interactions based on deep-layered learning. **M. Hamanaka***, K. Taneishi, J. Brown, Y. Okuno
- 11:15 – 334.** Strategy of structure generation within applicability domain. **H. Kaneko**, K. Funatsu*
- Sheraton Waikiki
Waianae
- Advances in Polymers for Medicine (#52)**
- Organized by: J. Pokorski, R. Advincula, T. Miyata, C. Boyer, K. Ishihara
Presiding: C. Boyer
- 8:00 – 335.** Shear-thinning, associative, and mucoadhesive hydrogels for improved eyedrop formulations. P. Sheikhholeslami, S. Mokhtari, B. Muirhead, D. Baek, H. Wang, X. Zhao, S. Boyd, H. Sheardown, **T. Hoare***
- 8:20 – 336.** Biodegradable injectable polymer formulation exhibiting temperature-responsive irreversible sol-gel transition by covalent bonds formation. **Y. Ohya***, Y. Yoshida, S. Mitsuhashi, A. Takahashi, A. Kuzuya
- 8:40 – 337.** Soft biomatter system based on cyocompatible polymers for advanced cell engineering. **T. Konno**
- 9:00 – 338.** Fabrication of decellularized aorta with electrospun fibers for small-diameter vascular grafts. **T. Kimura***
- 9:20 – 339.** Stimuli-responsive behavior of bioconjugated hydrogels, particles, and thin films with dynamic crosslinks. **T. Miyata***, A. Kawamura, T. Uragami
- 9:40 – 340.** Control of selectin-mediated cell adhesion on glycoprotein-conjugated matrices. **Y. Iwasaki**, A. Matsunaga, S. Fujii
- 10:10** Break
- 10:20 – 341.** Bioinspired and degradable protein-polymer conjugate therapeutics. **H. Maynard**, C. Decker, S. Paluck, T. Nguyen, E. Pellegrini-O'Day
- 10:50 – 342.** Nano-engineered polypeptide architectures and their potential applications in nano-medicine. **G.G. Qiao***
- 11:20 – 343.** Hydrogen sulfide-releasing micelles and their potential applications. **U. Hasegawa***, A.J. van der Vlies
- 11:40 – 344.** Nanofiber polyplex formation based on morphology elongation by intrapolyplex PEG crowding effect. **A. Harada***, K. Nomura, E. Yuba, K. Kono
- Hawaii Convention Center
Halls I, II, III
- Academic Drug Discovery (#69)**
- Organized by: J. Leahy, A. Mendonca, S. Hong, H. Kakeya, P. Scammells
Presiding: J. Leahy
- Poster Session**
- 10:00 – 12:00**
- 345.** Discovery of a potent anticancer agent from the optimization of natural oridonin scaffold. **J. Xu**, S. Xu, H. Yao
- 346.** Characterization of a Py-Im polyamide in models of castration resistant prostate cancer. **A. Kurmis**, F. Yang, N.G. Nickols, T.R. Welch, P.B. Dervan*
- 347.** Non-platinum-based halogenated compounds: A new class of potent antitumor agents for natural targeted chemotherapy of cancers. **Q. Zhang**, N. Ou, J. Warrington, C. Wang, Q. Lu
- 348.** Optimization of nitrofurazone cruzain and antitripanosomal activity by bioisosteric application. **G. Trossini***, D.G. Vital, F. Gatti, A. Andricopulo, V.G. Malterollo
- 349.** Isatin-dapsone based molecular hybrids as novel antimalarial and antitubercular agents. **M.M. Naseer***
- 350.** Rational design and optimization of drug leads and conformational antibody targeting pathological misfolding and aggregation of SOD1 enzyme in amyotrophic lateral sclerosis. **V.K. Hinge**, N. Blinov, N. Cashman, A. Kovaleko
- 351.** Development of novel therapeutics for the treatment of glaucoma. **P.I. Dosa***, M. Fautsch
- 352.** Host-based serine protease inhibitors as an emerging treatment against influenza. **P. Boudreault**, É. Colombo, P. Thakur, É. Gravel, I. Marois, D. Cliche, A. Cloutier, A. Griffin, B. Brown, M. Richter, R. Leduc, E. Marsault
- 353.** Exploration of the protein motion, allostery, and intra-molecular signaling pathways of GPCR activation, and its application to drug discovery. **S. Choi***
- 354.** Promising strategy to accelerate diabetic wound healing. **M. Gao**, T. Nguyen, M.A. Suckow, W.R. Wolter, H. Pi, S. Mobashery*, M. Chang*
- 355.** Design, synthesis, and structure-activity relationship studies of selective survivin inhibitors. **M. Xiao**, J. Wang, D. Miller, **W. Li**
- 356.** Rational design of novel spinogenic benzothiazoles for enhancing cognitive function. **J. Cifelli**, T. Chung, L. Dozier, H. Liu, M. Mayer, G. Patrick, J. Yang*
- 357.** Small-molecule inhibitor of MDM2 shows potent anticancer effect in a mouse leukemia model. **A. Dragaran**, L. Gu, H. Zhang, B. Wang*, M. Zhou
- 358.** Chemical diversification of pleurotinulin leads to discovery of a novel anticancer agent. **R.W. Hicklin**, E. Liblani, P.J. Hergenrother*
- 359.** Catalytic radical degradation by N-heterocyclic carbene-ruthenium complexes via a transfer hydrogenation-like process. **A.G. Tennison***
- 360.** Synthesis of coumarin derivatives possessing an inhibitory effect on aromatase. **M. Kawabata**, Y. Yamaguchi, N. Nishizono*, K. Oda*
- 361.** Holistic approach to collaborative drug discovery. **S. Ernst***
- 362.** Target identification of a HIF inhibitor using functional bioprobe. **K. Lee***, Y. Choi
- 363.** Design, synthesis, bioconversion, and pharmacokinetics evaluation of new ester prodrugs of olmesartan. **M.I. El-Gamal***, H.S. Anbar
- 364.** High-throughput drug discovery of novel inhibitors of secretion. **A. Satcho**, Y. Honjo, H. Suzuki, Y. Nishina
- 365.** ESI-MS probing of G-quadruplex DNA platinum(II) complex interactions. **D.L. Ang***, A. Craze, Y. Yuliani, C. Kelso, J.L. Beck, S.F. Ralph, D.G. Harman, J. Aldrich-Wright
- 366.** Quadruplex-DNA stabilising dinuclear platinum(II) complexes. **D.L. Ang***, D.G. Harman, S.F. Ralph, J. Aldrich-Wright
- 367.** Integrated flow and batch synthesis of 2-anilo substituted 3,4-dihydro-2H-benz[b][1,4]oxazine-6-carboxamides. **A.J. Lin**, A. McCluskey
- 368.** Chemical synthesis, plasmatic concentration, and antisulfatase activity in mice and rats of a tetrahydroisoquinoline derivative. **D. Poirier**, D. Ayan, R. Maltais, J. Roy
- 369.** Design and synthesis of conformationally restricted caprazamycin analogs as antibacterial agents. **M. Yamaguchi**, A. Matsuda, S. Ichikawa
- 370.** Discovery of novel and selective inhibitors of the Src homology-2 domain containing protein tyrosine phosphatase-2 (SHP2). **B. Czako***, P. Alessia, G. Liu, A. Yau, N. Reyna, R. Johnson, P. Leonard
- 371.** Data-driven drug design in the era of "Big Data". **M. Zheng***
- 372.** Novel N-(2,2'-disubstituted-2H-cromenyl)-N'-N'-disubstituted- guanidine derivatives as an S-nitroso glutathione reductase inhibitor. **S. Lim***, E. Kim*, G. Lee*, Y. Gong*
- 373.** Design, optimization, and synthesis of arylethynyl-substituted-heterocyclic compounds as trasnglutaminase 2 inhibitor. **N. Kim***, S. Kim, Y. Gong
- 374.** Synergistic antitumor effect of T-type calcium channel blockers and chemotherapeutic agents in human lung cancer. **B. PARK**, J. Nam, J. Lee*
- 375.** Computational structural analysis of 11β-hydroxysteroid dehydrogenase 1 through ensemble and induced fit docking studies to determine species difference. **S.J. Macalino**, S. Choi*
- 376.** Implications of auto-induction and heterotropic activation phenomena with cytochrome P450 enzymes: Examples of in vitro to in vivo translation from the neuroscience drug discovery field. **A. Blobaum***, F. Byers, T. Bridges, C. Niswender, C. Hopkins, C.W. Lindsley, J. Conn
- 377.** Synthesis and biological evaluation of 2-pyrrolidone derivatives as potent M₁ muscarinic acetylcholine receptor agonists. **M. Huang**, N. Cho, D. Bhattachari, S. Kang, A. Pae, H. Rhim, **G. Keum**
- 378.** Chemotherapy with hybrid liposomes without drugs along with induction of apoptosis in vivo. **H. Ichihara**, Y. Matsumoto*
- 379.** Synthesis and biological activity of phenylsulfonyl hydrazides for a potent suppressor of PGE₂ production. **E. Park**, **K. Kim**, J. Lee*
- 380.** N-(3-fluoro-4-methylsulfonylphenyl) ureas as potent TRPV1 antagonist. **J. Baek**, J. Ann, A. Jung, P.M. Blumberg, J. Lee
- 381.** Therapeutic effects of hybrid liposome against human carcinoma using model mice of carcinoma. **K. Kuwabara**, H. Ichihara, Y. Matsumoto*

*** Principle Author**

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TECHNICAL PROGRAM

- 382.** Diaza(bicyclic scaffold-based compounds: Using the hybrid approach for the development of new central nervous system drugs. **D. Guenidisch***
- 383.** Synthesis and *in vitro* antiproliferative activity of new pyrazole derivatives possessing diarylamide moiety. **M.M. Gamal Eldin, M.I. Elgamal, M.S. Abdel-Maksoud, Y. Kyung Ho, O. Chang Hyun***
- 384.** Catalytic asymmetric syntheses and biological evaluations of α -1-C-substituted L-imino furanose derivatives as α -glucosidase inhibitor. **Y. Natori, A. Kato, I. Adachi, Y. Yoshimura**
- 385.** In silico screening for selective inhibitors of SHIP2 as a novel therapeutic agent for diabetes. **S. Ozawa, H. Gouda, S. Hirono***
- 386.** Design and synthesis of α -arylidene DAG-lactones as selective RasGRP3 ligands. **j. Ann. N. Lewin, X. Zhou, P.M. Blumberg, j. Lee**
- 387.** Design, synthesis, *in vitro* antiproliferative evaluation, and kinase inhibitory effects of a new series of imidazo[2,1-*b*]thiazole derivatives. **M.S. Abdel-Maksoud, O. Chang Hyun, M. El-Gamal, M.M. Gamal Eldin**
- 388.** Design and synthesis of a non-zinc-chelating inhibitor selective for matrix metalloproteinase 13. **K. Mahasenan, M. Bastian, M. Gao, D. Ding, E. Frost, M. Chang*, S. Mobashery***
- 389.** Synthesis and biological comparison of enantiomers of mepenzolate bromide, a muscarinic receptor antagonist with bronchodilatory and anti-inflammatory activities. **Y. Yamashita, T. Mizushima**
- 390.** Design, discovery, and one-pot, multi-component Bi(NO₃)₃ catalysed synthesis of novel monastrol-1,3,5-triazine conjugates targeting Rad6B as antiproliferative agent with antibacterial and antifungal activity. **U.P. Singh*, J.K. Srivastava, H.R. Bhat**
- 391.** In silico study on the interaction of high affinity ligand calystegine B₂ with β -glucocerebrosidase. **I. Nakagome***, A. Kato, T. Yoshida, N. Yamaotsu, I. Adachi, S. Hirono
- 392.** Macrocyclic phosphopeptidomimetics as inhibitors of the polo-box domain of polo-like kinase 1. **D.L. Kuncic***, C. De Fusco, J. Fuchs, M. Rossmann, A. Bender, M. Hyvonen, D. Spring
- 393.** Therapeutic effects of hybrid liposomes against colon carcinoma using xenograft mouse models of colon carcinoma. **M. Okumura, H. Ichihara, Y. Matsumoto***
- 394.** Inhibitory effects of liposomes including trehalose surfactants on the growth of tumor cells along with apoptosis. **M. Kuwano**, H. Ichihara, Y. Matsumoto*
- 395.** Diversity-oriented synthesis of anti-inflammatory and cytotoxic 4-hetero-2-cyclopentenones. **A.C. Macabeo*, P. RUBIO, J. TIU, A. VERANO, I. SORNE**
- 396.** Finding the sweet spot: Structure-based design of Hsp90 inhibitors and their effects against drug-resistant cancer cells. **Y. Seo***
- 397.** Three new prenylated indole alkaloids from *Aspergillus taichungensis* (IBT 19404). **I. Kagiyama, H. Kato, S. Tsukamoto***
- 398.** Discovery and SAR of a novel series of selective negative allosteric modulators of the metabotropic glutamate receptor subtype 2 derived from a substituted tetrahydroquinoline core. **A. Felets***, K. Smith, A. Rodriguez, R. Morrison, S. Daniels, C. Niswender, J. Conn, C.W. Lindsley, K. Emmitt
- 399.** SOAT inhibitory activity and antiatherogenic activity of beauveriolide derivatives. **T. Ohshiro***, S. Imuta, I. Hijikuro, T. Takahashi, T. Doi, H. Tomoda*
- 400.** Progress toward the X-ray crystal structure of TREM2, a protein involved in Alzheimer's disease. **A. Sens, H. Ng***
- 401.** High-throughput screening for the discovery of novel inhibitors to mitigate ruminal methane emissions. **L.R. Schofield***, Y. Zhang, C. Sang, R. Atua, S. Molano, A. Beattie, D. Dey, G. Cook, J. Cheung, Y. Kobayashi, W. Whitman, C. McSweeney, M. Morrison, W. Denny, A. Sutherland-Smith, V. Carbone, R. Ronimus
- 402.** Targeting bioactive chemical space with a small natural products library: Expanding diversity and predictability. **J.L. von Saml-Fries***, D. Santiago, N.G. Wilson, L. Calculi, D.E. Kyle, W.C. Guida, B. Baker
- 403.** Chemical probes for drug development and target identification in amyotrophic lateral sclerosis. **K.T. Zhao, I.T. Schieffer, R.B. Silverman**
- 404.** Screening for FtsZ dimerization inhibitors using several evaluation systems including in dry and wet. **K. Kodama, S. Mikiuri, A. Sasaki, N. Kohira, H. Maki, M. Munetomo, K. Maenaka, M. Kinjo**
- 405.** Development of WNK signaling inhibitors as new class of antihypertensive drugs. **M. Yuasa, T. Mori, S. Fujii, Y. Watanabe, H. Suzuyama, E. Kikuchi, Uchida, H. Kagechika***
- 406.** Study of substituted stilbenes and flavonoids as replication inhibitor of hepatitis C virus. **A. Nag*, U. Ononuju, T. Hansberry II, N. Mateeva**
- 407.** Development of a PARP-inhibiting boron tracedrug for neutron dynamic therapy. **R. Tada*, H. Yamada, E. Nakata, K. Masuda, T. Morii, Y. Uto**
- 408.** Identification of novel small molecules for kidney disease. **E. Grimley, C. Liao, E. Ranghini, Z. Nikolovska-Coleska, G. Dressler**
- 409.** Improved synthesis and mechanistic study of a radiosensitizer, sulfoquinovosyldiacylglycerol (SQAG) derivatives. **Y. Sawamoto, t. tanaka, M. Umezawa, Y. Hisamatsu, I. Tamai, K. Sakaguchi, S. Aoki**
- 410.** Design and synthesis of novel 2,4-diaminopyrimidine analogs for anaplastic lymphoma kinase (ALK) inhibitor. **J. Ha*, J. Hwang, C. Park, C. Lee, C. Yun, H. Jung, P. Kim, S. Cho, H. Kim**
- 411.** Development of novel activators for transcriptional co-activator TAZ involved in Hippo pathway. **A. Dilihuama, S. Ito, K. Nakagawa, Z. Yang, M. Yuasa, Y. Hata, H. Kagechika**
- 412.** Synthesis of chromone and coumarin derivatives possessing an inhibitory effect on human CYP2A6. **Y. Yamaguchi, N. Nishizono*, S. Toyota, D. Kobayashi, T. Yoshimura, K. Wada, K. Oda***
- 413.** Design, synthesis, and biological evaluation of novel rosamine derivatives as inhibitor of tau aggregation. **Y. Yu, Y. Chang, Y. Kim*, H. Ha***
- Sheraton Waikiki
Waialua
- Nutraceuticals and Functional Food Ingredients: Chemistry and Health (#285)**
- Organized by: F. Shahidi, C. Ho, R. Pegg, K. Miyashita
Presiding: K. MIYASHITA, R.B. Pegg, F. Shahidi
- 8:00 Opening**
- 8:05 – 424.** Novel antioxidant activity of sphingoid base on omega-3 fish oil. **K. MIYASHITA, M. Uemura, A. Suzuki, M. Shiota, M. Hosokawa**
- 8:25 – 425.** Membrane lipid peroxidation in human nutrition and aging. **T. Miyazawa**
- 8:45 – 426.** Enhancing solubility of bioactive lipid agents. **C.T. Le*, M. Arella, M. Mateescu**
- 9:05 – 427.** Evaluation of biological activities of marine carotenoids for nutraceuticals. **T. Sugawara**
- 9:25 – 428.** Green approach for extraction of bioactive nutraceuticals from marine macroalgae. **A.T. Quaitan***, M. Sasaki, T. Kida
- 9:45 break**
- 9:55 – 429.** Extraction of 7-hydroxymatairesinol from Norway spruce knots using ionic liquids aqueous solutions. **A. Ferreira*, A. Leite, J. Coutinho, B. Holmbo, T. Holmbo, M.G. Freire, A. Silvestre**
- 10:15 – 430.** Safety and efficacy of a novel *Prunus domestica* extract (CR002) on testosterone-induced benign prostatic hyperplasia (BPH) in male Wistar rats. **D. Bagchi*, A. SWAROOP, M. Bagchi**
- 10:35 – 431.** Phytochemicals as agonists of nuclear hormone receptors: The case for soy isoflavones. **N.F. Shay*, t. Iuo**
- 10:55 – 432.** Anthocyanins profile of Quebec wild blueberries, their oxygen radical absorbance capacity, and *in-vitro* human LDL oxidation inhibition effect. **K. Belkacemi*, N. Chorfa, S. Savard**
- 11:35 Closing**
- 11:15 – 433.** From a sweetener to fighting gut inflammation. **Y. Mine***
- Hawaii Convention Center
Halls I, II, III
- Bench to Bedside: Chemistry of Health Care General Posters**
10:00 – 12:00
- Miscellaneous drug and vivo activities**
- 434.** Retrospective assessment of organophosphorus nerve agent exposure in humans. **R.N. Harding*, T.H. Corzett, A.M. Williams***
- 435.** Influence on the bone strength due to mineral administration to osteoporosis model mouse. **A. Arakaki, A. Onodera, H. Yasui, Y. Yoshikawa**
- 436.** Exploration of predictive blood biomarkers of the cat chronic kidney disease. **Y. Matsumura*, A. Iwasawa, T. Yoshida, K. Azuma, Y. Okamoto, N. Ito**
- Drug Delivery, Devices, Formulations and Instrumentation**
- 437.** Development of a laser irradiating device for hemostasis in neuroendoscopic surgery. **T. Seki*, K. Oku*, H. Akutsu***
- 438.** Block copolymers encapsulated dendrimer silicon (IV) phthalocyanine for *in vivo* photodynamic efficacy of choroidal neovascularization. **Z. Chen*, H. Lu, X. Yu, S. Pan, J. Wen, Z. Huang, Y. Peng***
- 439.** Influence of the condensation in the heat and moisture exchangers (HME) on the measurement of temperature and humidity. **R. Fujiwara, T. Narisawa, Y.asaki, A. Yamashita, S. Ohwaki, M. Kamiya**
- 440.** Comparative phantom study on the spatial resolution of a small animal PET scanner using ¹¹C, ⁶⁸Ga, ¹⁸F, ⁶⁴Cu, ⁶⁹Zr, and ⁴⁴Sc. **M. Bunka*, S. Haller, N. van der Meulen, R. Schibli, A. Türler, C. Müller**
- 441.** Influence of the membrane surface area and other design factors on the performance of the dialyzer. **Y. Aizawa, Y. Yamada, A. Yamashita**
- 442.** PEO-silane amphiphiles to reduce biological adhesion onto silicone medical devices. **M.A. Grunlan**
- 443.** Single-wall carbon nanotubes-dendrimer zinc (II) phthalocyanine nanocomposites: Synthesis and photophysical properties. **J. Wen, X. Yu, H. Lu, S. Pan, Z. Huang, Y. Peng***
- 444.** Effect of substitution position on the photophysical property of polymer nanoparticles encapsulating aluminium phthalocyanines. **K. Chen, J. Wen, D. Ma, Z. Huang, Y. Peng* Modeling and QSAR**
- 445.** Application of cifar for predicting the binding affinity of chk1 inhibitors derived from 2-aminothiazole-4-carboxamide. **O. Erdas*, D. Konyar, F. Alpaslan, E. Buyukbingol**
- 446.** Amino acid residue-based 3D-QSAR analysis using PLS regression and FMO calculation. **T. Yoshida, S. Hirono**
- 447.** mRNA structure prediction targeting antisense oligonucleotides (AONs). **M. Yamashita, N. Kawashita, T. Yamamoto, K. Okamoto, T. Takagi*, S. Obika**
- 448.** Molecular docking study of phytochemical estrogen mimics from dietary herbal supplements. **C.N. Powers, W.N. Setzer***
- 449.** Novel telomerase inhibitors for cancer therapy - *in silico* design and biological evaluation. **M. Padaraya, U. Kalathiyia, M. Wysocka, M. Serocki, A. Skladanowski, M. Baginski***
- 450.** Molecular modeling studies of neurokinin-1 receptor antagonists. **O. Ozturk*, T. Ertan-Bolelli, K. Bolelli, S. YILMAZ, I. Yalcin, E. Aki-Yalcin**
- 451.** Molecular docking studies of some new benzothiazole derivatives on human glutathione-S-transferase enzyme. **T. Ertan-Bolelli*, K. Bolelli, Y. Musdal, B. Mannervik , E. Aki-Yalcin, I. Yalcin**
- 452.** Common feature pharmacophore generation of hGST P1-1 enzyme inhibitory active benzazole derivatives. **K. Bolelli*, I. Yalcin, T. Ertan-Bolelli, S. YILMAZ, O. Ozturk, E. Aki-Yalcin**
- 453.** Development of novel fluorescent retinoid X receptor antagonists using RXR antagonist NEt-SB as a lead compound. **S. Yamada, M. Nakayama, M. Makishima, H. Naitou, H. Kakuta***

* Principle Author

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<http://pacifichem.org/onlineprogram>

454. Molecular docking studies of some novel bacterial topoisomerase II inhibitors. **S. YILMAZ***, T. Ertan-Bolelli, K. Bolelli, O. Ozturk, E. Aki-Yalcin, I. Yalcin

Medicinal Chemistry

455. Discovery of novel liver X receptor antagonists from cinnamamide derivatives as potential therapeutics for nonalcoholic fatty liver disease. W. Sim, D. Kim, K. Shin, H. Park, **B. Lee***

456. Design, synthesis, and biological evaluation of annulated 1,7-diarylhepta-1,6-diene-3,5-diones as curcumin analogs. **A. Jha**

457. Bioactivity of isohexenylnaphazarins from root extracts of *Echium* spp. in native and invaded ranges. **A. G. Duran**, **D. Skoneczny**, A. Torres, M. M. Valdivia, J.M. G. Molinillo, L.A. Weston, F.A. Macias

458. Oxopyrido[2,3-d]pyrimidinyl derivatives as irreversible epidermal growth factor receptor (EGFR) inhibitors with improved selectivity for the L858R/T790M mutant over wild-type. **R.P. Wurz***, L. Pettus, J. Zhan, P. Mitchell, K. Cooke, T. Wu, D.L. Reid, R. Radinsky, P. Beltran, A.S. Tasker

459. Matrix metalloproteinase-3 accelerates healing of both the diabetic and nondiabetic wound healing. **T.T. Nguyen**, M.A. Suckow, W.R. Wolter, H. Pi, S. Mobashery*, M. Chang*

460. Therapeutic effects of novel retinoid x receptor partial agonist CBT-PMN on cognitive impairment in mice. T. Kobayashi, **O. Shibahara**, Y. Furusawa, T. Sasaki, M. Akehi, S. Yamada, M. Fujihara, M. Nishii, H. Kakuta

461. Degalactosylated/desialylated human serum and bovine colostrum induces macrophage phagocytic activity. **Y. Uto**, H. Yamada, D. Kuchikie, T. Inui, T. Inui, M. Mette, K. Tokunaga, A. Hayakawa, A. Go, T. Osaki

462. Side selective covalent attachment of heparin to PES hollow fiber membranes to enhance collection of heparin-binding proteins. **S. Phillips**, J. Stenken

463. Elucidation of the reason for less side effects of retinoid X receptor full agonist NEt-3IB than bexarotene. T. Kobayashi, **S. Nakatani**, Y. Furusawa, M. Watanabe, M. Nishi, M. Fujihara, S. Yamada, H. Kakuta*

464. Antibacterial glycosides: Bioactivity and toxicity. **J.A. Justino***, A. Rauter, A. Martins, C. Dias, R. Nunes, J.P. Pais, A. Almeida, P. Serra

465. New 5'-O- and 6-substituted purine nucleoside analogs: Synthesis and cytotoxic activity on selected human cancer cell lines. **D. Sac***, M. TUNCBILEK, I. DURMAZ, R. Cetin-Atalay

466. Antiprototrophic activity of newly synthesized mono/dicationic benzimidazole carboxamides derivatives. **C. Karaaslan***, H. Goker, R. Brun

467. MYC promotes coupling of energetic nutrient utilization to nucleotide biosynthesis via de novo amino acid synthesis. **A.N. Lane***, T.W. Fan, A. Le, Z.E. Stine, P.P. Shah, L.J. Beverly, Y. Yang, K.I. Zeller, W. Zhou, H. Ji, R.M. Higashi, C.V. Dang

468. Discovery and development of small molecule inhibitors toward the Chikungunya virus. K. Ching, J.Y. Kam, L.F. Ng, **C.L. Chai**

469. Preparation and structural characterization of the samarium EDTMP complex employed in palliative treatment of bone metastases. **J.M. Pushie***, Y. Yang, D.M. Cooper, M. Doschak

470. Therapeutic effect on inflammatory bowel disease of RXR full agonist NEt-3IB which is hardly absorbed by oral administration. Y. Furusawa, T. Kobayashi, **M. Watanabe**, K. Morishita, M. Nishi, M. Fujihara, S. Nakatani, O. Shibahara, S. Yamada, H. Kakuta*

471. Sulfur hot spring water containing hydrogen generated by UV light irradiation. **Y. Mukae**, K. Umeha, Y. Kurita, H. Niihara, S. Okouchi, A. Tsuneshige

472. Effects of magnesium hydride as a reductive bath additive for the skin. **Y. Kurita**, Y. Mukae, K. Umeha, A. Tsuneshige, S. Okouchi

473. Research supporting platform for academic drug discovery in Japan. **H. Kojima***, T. Okabe, H. Ichijo, T. Nagano

Friday Afternoon

Sheraton Waikiki
Lanai

De Novo Drug Design (#28)

Organized by: G. Schneider, D. Winkler, K. Funatsu, Y. Okuno
Presiding: Y. Okuno, D. Winkler

13:00 – 474. Drug designs by large-scale molecular dynamics simulations using a special purpose computer. **M. Taiji***, I. Ohmura, G. Morimoto, Y. Ohno, A. Hasegawa, N. Okimoto, Y. Hirano, T. Otsuka

13:40 – 475. Creating a very large-scale virtual library for drug discovery. **A. Hasegawa***, Y. Fujihara, G. Morimoto, Y. Hirano, N. Okimoto, M. Taiji*, K. Funatsu

14:10 – 476. Development of the protein-gene sequence motif analysis system based on the codon reduced representation. **H. Kato***, J. Yamamoto

14:40 Break

15:00 – 477. Computer-aided lead optimization, synthesis, and protein crystallography for biaryltriazoles as inhibitors of macrophage migration inhibitory factor. **W.L. Jorgenson***, P. Dziedzic, J.A. Cisneros, M.J. Robertson

15:40 – 478. Development of dengue virus NS2B/NS3 protease inhibitor by ligand-based virtual screening. **N. Kawashita***, S. Pambudi, Y. Tian, K. Ikuta, K. Takeshi, T. Takagi

16:10 – 479. Characterization of hydration properties of ligand binding sites with the 3D-RISM-KH molecular theory of solvation. **N. Blinov***, A. Kovaleko

16:40 Closing Remarks

Sheraton Waikiki
Waianae

Advances in Polymers for Medicine (#52)

Organized by: J. Pokorski, R. Advincula, T. Miyata, C. Boyer, K. Ishihara
Presiding: K.L. Lee, J. Pokorski

13:00 – 480. Bioactive polysaccharide-based pH-sensitive polymers for cytoplasmic delivery of antigen and activation of antigen-specific immunity. **E. Yuba**, A. Yamaguchi, A. Harada, K. Kono*

13:20 – 481. Novel cancer vaccine using peptide/CpG-DNA/β-1,3-glucan complex. **S. Mochizuki***, H. Morishita, K. Sakurai

13:40 – 482. Highly efficient, directional mucosal drug delivery system by employing Janus patch. **S. Im***, K. Lee, J. You

14:00 – 483. Aluminium phthalocyanine incorporating nanoparticles: Photophysical property, size, and in vitro photodynamic therapy efficacy. S. Pan, Z. Chen, J. Wen, D. Ma, Z. Huang, **Y. Peng***

14:20 – 484. Improving cellular uptake of siRNA: Native chemical ligation of cell penetrating peptides to polymeric siRNA delivery vectors. **E.G. Williams***, F. Louvet de Verchere, P. Duggan, O. Hutt, G. Thilak, T. Hinton, T. Le, S. Thang, X. Nguyen

14:40 – 485. Development of a virus-based stealth filament for cancer therapy. **K.L. Lee**, S. Shukla, K. Weber Bonk, R.A. Keri, N.F. Steinmetz

15:00 Break

15:20 – 486. Combating thrombosis and infection with nitric oxide (NO)-releasing polymers. **E.J. Brisbois**, T. Major, J. Wu, H. Handa, R. Barletta*, M.E. Meyerhoff*

15:40 – 487. Characterization of a chitosan/dextran-based surgical hydrogel for protein and stem cell delivery. **J. Cabral***, M. McConnell, E. Mathis, E. Tan, J. Faed, L. Hanton, S.C. Moratti

16:00 – 488. Bubble elimination with a temperature-responsive polymer for cell culture. **N. Tanaka***, Y. Tanaka

16:20 – 489. Chitosan composites encapsulating cellobiose dehydrogenase: An antimicrobial system for wound applications. **G. Tegli***, B. Thallinger, B. Beer, G.S. Nyanhongo, G.M. Guebitz

Sheraton Waikiki
Maui

Academic Drug Discovery (#69)

Organized by: J. Leahy, A. Mendonca, S. Hong, H. Kakeya, P. Scammells
Presiding: H. Kakeya

13:00 – 490. Academic drug discovery: A growing role in advancing biomedical research and sustaining healthcare. **R.N. Young***

13:30 – 491. Building a pipeline - drug discovery at Rethna Deaconess Medical Center. **L. Sun**

13:50 – 492. Electron-transfer-based combination therapy of cisplatin with a molecular promoter for cancer treatment. **Q. Zhang**, N. Ou, Q. Lu

14:10 – 493. Developing photoswitchable tools for manipulating the activity of native neuronal systems with light. **H. Schoenberger**

14:30 – 494. Developing small molecules targeting Gli-2,3 transcription factors as cancer suppressing agents. **N. TRINH***, I. Bernstein, C. Gordon, E. McLaughlin, A. McCluskey

14:50 – 495. Soluble epoxide hydrolase (sEH) inhibitors have high target engagement and block neuropathic pain. **B. Hammock**

15:15 – 496. Mitotic kinase inhibitors of novel structure as potent anticancer agents: Case studies from academia. **H.W. Pauls***

15:40 – 497. Drug discovery in academia: A successful case study. **M.E. Jung**

16:20 – 498. CPP-115: A novel GABA amionotransferase inactivator and potential new treatment for multiple indications. **R.B. Silverman***

Sheraton Waikiki
Oahu

Chemistry of Molecular Imaging (#215)

Organized by: H. VanBrocklin, G. Tamagnan, Y. Fujibayashi, L. Luyt, A. Katsifis, Y. Choe, N. Vasdev
Presiding: V.N. Carroll, L. Luyt

13:00 – 499. Molecular imaging with high aspect ratio, protein-based, macromolecular MRI contrast agents. **N.F. Steinmetz**

13:35 – 500. Hybrid polarizing solids for pure hyperpolarized liquids through dissolution dynamic nuclear polarization. **D. Gajani***, A. Bornet, B. Vuichoud, J. Milani, R. Melzi, H. Van Kakeren, L. Veyre, C. Thieuleux, M. Conley, W. Gruning, M. Schwarzwälder, A. Lesage, C. Copéret, G. Bodenhausen, L. Emsley, S. Jannin

13:55 – 501. Synthesis and functional evaluation of novel chiral dendrimer-triamine-coordinated Gd complexes as a highly sensitive MRI contrast agent. **Y. Miyake**, Y. Kimura, T. Matsuda, H. Imai, A. Toshimitsu, T. Kondo

14:15 – 502. Schiff-base macrocycles as a platform for small molecule-based bi-modal MRI contrast agents. **M. Pilkington***

14:35 – 503. Bimodal nanoassemblies for cell tracking and ultrasensitive detection. A. Faucon, S. Nedellec, P. Hulin, H. Benhelli-Mokrani, F. Fleury, M. Tramier, S. Dutertre, F. Gauffre, L. Lartigue, E. Ishow

14:55 Break

14:55 – 514. Preparation of hydroxyapatite/collagen composite from grass carp scale. P. Tsai, Y. Wang, T. Lin, **C. Kuo**

15:15 – 515. Cyclin D1 proteasomal degradation by kahweol as the molecular target for cancer chemoprevention. **G. Park***, J. Jeong

15:35 – 516. Inhibitory effect of silymarin on Wnt signaling through downregulation of β-catenin and TCF-4 in human colorectal cancer cells. **H. Eo***, J. Jeong

15:55 – 517. Identification of benzyl isothiocyanate-targeted genes using a yeast screening system. **N. Abe***, N. KUNISUE, S. Munemasa, Y. Murata, A. Satoh, H. MORIYA, Y. Nakamura

16:15 – 518. Dysthymia and S-adenosyl-L-methione. **A. Stergiou***, G. Uechi, N.D. Sachinvala

16:35 – 519. Enzyme-assisted extraction of anticoagulant polysaccharide from *Liparis tessellatus* eggs. **B.F. Ticar***

* Principle Author

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16:55 closing

Friday EveningHawaii Convention Center
Halls I, II, III**Nutraceuticals and Functional Food Ingredients: Chemistry and Health (#285)**

Organized by: F. Shahidi, C. Ho, R. Pegg, K. Miyashita
Presiding: C. Ho, K. MIYASHITA, R.B. Pegg, F. Shahidi

Poster Session
19:00 – 21:00

520. Betulinic acid supplementation reduces lipid accumulation in differentiated 3T3-L1 adipocytes via a SREBP1-related pathway. **G. Go***

521. Cyclic GMP as a critical signal mediator for green tea polyphenol epigallocatechin-3-O-gallate through the sensing receptor 67LR. **H. Tachibana**

522. Phytochemical content and antidiabetic properties of *Aloe ferox* and *Aloe great-headii* var. *davyana*. **M. Pieters***, D. Loots

523. Effects of methanol extracts of traditional Okinawa vegetables on the activation of antigen-presenting cells J774.A1) and histamine release from KU812 cells. **J. Nagata***, T. Matsuzoe, S. Aono, G. Maeda

524. Engineering anti-listerial Class IIa bacteriocin Leucocin A for application in food storage. **K. Kaur**, M. Stiles, R. Dargeti

525. Hypolipidemic effect of orally administered Oligonol, a low-molecular-weight polyphenol derived from lychee fruit, in rats fed diet with lard. **K. Hayashi, S. Kawai, K. Hinohara, K. Osada***

526. Evaluation of the action of the solvent molecules to the weak interaction between the large-sized γ -cyclodextrin and the chiral lipoic acid. **M. Doe***, K. Nishikawa, Y. Tachi, Y. Morimoto

527. Effects of Uva tea on α -glucosidase activity and blood glucose levels. **N. Takamizawa***, A. Nakamura, M. Moto, K. Katsumura, K. Yazawa

528. Comparison of flavan-3-ols components on the sympathetic nerve stimulation activity. **Y. Nakagawa***, K. Ishimura, S. Abe, N. Osakabe

529. Anti-inflammatory effects of extracts from *Chaenomeles sinensis* leaves on RAW264.7 macrophages. **N. Jeon**, Y. Kim, J. Hwang, S. Kim, B. You, X. Dong, P. Park

530. Purification and characterization of a compound from *Umbellaria esculenta* and evaluation of its antioxidative property. **X. Dong**, Y. Kim, J. Hwang, S. Kim, B. You, N. Jeon, P. Park

531. Piperine enhances glucose uptake through AMPK signaling pathway in skeletal muscle. **A. Maeda**, M. Akagawa, Y. Yamashita, H. Ashida*

532. Characterizations of a novel heteropoly-saccharide isolated from seeds of *Plantago asiatica* L. and its anti-inflammatory activities. **Y. Niit***, L. Gong, S. Alaxi, L. Chen, L. Yu

533. Procyanidin promotes translocation of glucose transporter 4 in muscle of mice through activation of insulin and AMPK signaling pathways. **Y. Yamashita**, H. Ashida

534. Role of phosphate groups on anti-FCV activity of casein phosphopeptide. **N. LEBETWA***, S. Katayama, S. Nakamura

535. Anticancer effect of thymol on AGS human gastric carcinoma cells. **P. Park**, Y. Kim, J. Hwang, S. Kim, B. You, N. Jeon, X. Dong

536. Physicochemical characteristics of a high molecular weight biogenerered α -D-glucan from *Leuconostoc citreum* SK24.002. **M. Miao**, B. Jiang

537. Potential of microalgae as a novel cosmetic ingredient. **S. Kamako***

538. Anti-hyperglycemic compounds isolated from Acer spp. **Y. FU***, A. Honma, T. Ohshima, T. Koyama*

539. 4-Hydroxyderricin and xanthoangelol from Ashitaba (*Angelica keiskei*) suppress differentiation of preadipocytes to adipocytes via AMPK and MAPK pathways. **H. Ashida**, T. Zhang, Y. Yamashita, N. Yamamoto

540. Effects of dietary whey protein on the body fat-reducing potential of conjugated linoleic acid in rats. **K. Koba***, S. Tamaru, M. Hirata, Y. Arimoto, K. Kawabeta, T. Noda, N. Tateiwa, S. Matsuda, T. Iwata

541. Immunological tolerance effects of attenuated buckwheat allergens prepared by dry-heating with pyrophosphate. **D. Yamaguchi**, S. Katayama, S. Nakamura

542. Antidiabetic effect of hijiki with lower-molecular-weight fucoxidin in type 2 diabetes model KK-A^y mice. **A. Nakamura***, M. Moto, N. Takamizawa, K. Katsumura, K. Iwasaki, K. Tanaka, A. Murota

543. Phenolic compounds and anti-oxidant capacities of the whole grain rice from China. **X. Liu**, L. Ye, S. Zhou

544. Mung bean protein isolate improves glucose tolerance by enhancing glucose transporter 4 translocation and glucose uptake in skeletal muscle. **X. Wang**, Y. Yamashita, N. Tachibana, S. Wanazaki, M. Kohno, H. Ashida

545. Effect of olonghomobisflavan on chemical mediators release from mast cells. **H. Arai***, K. Toda, E. Sukhbold, L. Yang, M. Takasugi

546. Evaluation of freshness of fermented foods by aging index criterion: A case for yogurt. **Y. Hattori***, Y. Kunta, T. Suzuki, S. Okouchi, A. Tsuneshige

547. Screening for a candidate agent capable of inducing immune tolerance using TGF- β secretion system from dendritic cell. **F. Ohno**, S. Katayama, S. Nakamura

548. Effect of oral ingestion of wheat peptide on enterocyte turnover during methotrexate-induced intestinal mucositis in rats. **B. Yan**, I. Liu, S. Zhou

549. Effect of steam explosion-assisted extraction on phenolic acid profiles and antioxidant properties of wheat bran. **I. Liu***

550. Regulating role of nuclear factor-kappaB in benzyl isothiocyanate-induced antiproliferation in p53-deficient colorectal cancer cells. **N. Abe**, D. Hou, S. Munemasa, Y. Murata, **Y. Nakamura***

551. Comparing the effect of temperature and pH on the stability of betalains from beetroot and dragon fruit. **M.I. Hashmi***, K. Ruying, B. Rasti

552. Large scale growth of *Haematococcus pluvialis* for astaxanthin production using a semi-continuous culture system. **G.L. Wagner***

553. Hepatoprotective activity of *Momordica charantia* water extract in stress mice. **Y. Deng***, Y. Zhang, R. Zhang, Z. Wei, H. Ti, L. Liu, M. Zhang

554. Anti-atherosclerotic activity of litchi pericarp procyanidins and the mechanism of nf- κ B inhibition. **R. Zhang***, H. Ti, Y. Deng, L. Liu, Y. Zhang, Z. Wei, M. Zhang*

555. Characterization and quantification of phenolic compounds of *Tetrastrigma hemisleyanum* by a combination of UPLC-QTOF-MS and UPLC-QQ-MS and their antioxidant/antiproliferative activities. **Z. Deng***

556. Intestinal absorption and bioactivity of ginsenoside Rh2 and its esterification derivative. **J. Hu***, B. Zhang, Z. Deng

557. Antihypertensive effects of choline esters in fermented foods. **K. Nakamura***, M. Koyama, N. Igari

558. Carotenoid from green algae effectively suppresses mast cell degranulation via an alteration of cellular sphingomyelin metabolism. **Y. Manabe**, T. Hirata, T. Sugawara*

Saturday Morning

Sheraton Waikiki

Maui

Academic Drug Discovery (#69)

Organized by: J. Leahy, A. Mendonca, S. Hong, H. Kakeya, P. Scammells
Presiding: A. Mendonca

8:00 – 559. Academic drug discovery and chemical biology: A tale of two targets. **S.V. Frye***

8:30 – 560. Design and discovery of PW73597 (VDC-597), a dual inhibitor of PI3-kinase alpha and mTOR. **G.W. Rewcastle***, A. Giddens, J. Flanagan, S.A. Gamage, S.K. Tsang, J.D. Kendall, B.C. Baguley, C.M. Buchanan, D.J. Matthews, M. O'Farrell, S. Jamieson, W. Denny, P.R. Shepherd

8:50 – 561. Click-and-release approach to CO prodrugs. **B. Wang**

9:10 – 562. Natural product inspired fragment-based drug discovery: Development of inhibitors of *M. tuberculosis* CYP121 inhibitors. **M.E. Kavanagh**, J. Gray, A.G. Coyne, H. Davis, K. McLean, A.W. Munro, C. Abell

9:30 – 563. Small molecule control of intracellular protein levels: A therapeutic strategy. **C.M. Crews***

10:10 – 564. Discovery of Trofinetide (NNZ2566) - the first drug for Rett syndrome. **M.A. Brimble**

10:40 – 565. Invention of SAHA and some related more selective compounds. **R. Breslow***

Hawaii Convention Center

Halls I, II, III

Small Molecule Epigenetic Modulators (#146)

Organized by: C. Burns, P. Brown, S. Frye

Poster Session**10:00 – 12:00**

566. Relevant epigenetic chemical space: A chemoinformatic characterization of small molecules – DNMT inhibitors. **E. Fernández de Gortari***

Sheraton Waikiki
Waianae

In Vivo Chemical Strategies for Functional and Translation Studies of Biological Networks and Pathways (#212)

Organized by: M. Bogyo, K. Kikuchi, B. Cravatt, H. Kwon

8:00 – 567. Activity-based proteomics – applications for enzyme and inhibitor discovery. **B.F. Cravatt***

8:30 – 568. New chemical probe technologies for diagnostic and intra-operative imaging applications. **M. Bogyo**

9:00 – 569. Differential scanning calorimetry as a new tool for biomarker research. **N.C. Garbett**, M. Granger-Delacoux, N.C. Allen, A. Kalilappan, M.L. Merchant, D.M. Miller, J.A. Chesney

9:20 – 570. Ribonuclease: From k_{cat}/K_m to the clinic. **R.T. Raines***

9:50 – 571. daVinci surgical system and other platforms for the clinical translation of molecular imaging agents. **J. Sorger***

10:20 break

10:30 – 572. Small-molecule inhibitors of Gli transcription factor function. **A. Ondrus, T. Sakata-Kato, J.K. Chen***

11:00 – 573. Rationally designed activatable fluorescence probes appropriate for assisting interventional and theranostic procedures. **H. Kobayashi***

Sheraton Waikiki
Lanai

Molecular Design in Medicine: Concept to Commerce (#295)

Organized by: J. Siegel, M. Martinelli, M. Brimble, M. Platz, H. Wong, K. Baldridge
Presiding: K. Baldridge

8:00 Speaker Prep

8:15 – 574. Importance of molecular design in the development of new platform analytical and purification tools for pharmaceutical discovery and development. **C. Welch**

8:40 – 575. Designing potential new medicines. **M.E. Jung**

9:05 – 576. Chemical discovery through a computational lens. **R. Amaro***

9:30 – 577. Targeting key apoptosis regulators for new cancer therapeutics: From discovery to clinical development. **S. Wang**

9:55 – 578. Drug design based on ligand-target binding thermodynamics and kinetics. **H. Jiang***

10:20 – 579. Meeting the challenge of F18 labeling through molecular design to create a new class of PET imaging agent for clinical applications. **D. Perrin**, Z. Liu, R. Ting, K. Lin, F. Benard

10:45 – 580. Medicinal chemistry challenges and opportunities using phenotypic assays. **D.M. Huryn***

11:10 – 581. QSAR on biomolecular interaction. **Z. Xi**

11:35 – 582. Asymmetric total synthesis of (–)-Lingzhiol via a novel type of Rh-catalyzed [3 + 2] cycloaddition. **Z. Yang***

Sheraton Waikiki
Oahu

Non-canonical Approaches to 18F-labeling: New Frontiers in Stable Non-carbon-fluorine Bonds (#337)

Organized by: D. Perrin, F. Gabbari, F. Li, R. Schirrmacher

7:55 Break

8:00 – 583. One-step 18F-labeling of peptides and other complex biologics. **D. Perrin***, Z. Liu, K. Lin, F. Benard

8:20 – 584. Application of the ^{18}F - ^{19}F isotope exchange reaction on an ammonium trifluoroborate moiety for the design of cancer-targeting PET tracers. **K. Lin***, J. Pan, Z. Zhang, J. Lau, S. Jenni, N. Hundal-Jabal, N. Colpo, Z. Liu, D. Perrin, F. Benard

8:40 – 585. Silicon fluoride acceptors (Si-FAs): From bench toward bedside. **R. Schirrmacher***

9:20 – 586. Radiotracerization of pre-formed group 13 aza-macrocyclic complexes - toward next generation PET imaging agents. **R. Bhalla, W. Levason, S. Luthra, G. Robbie, G. Reid*, G. Sanderson**

10:00 Break

10:10 – 587. Labeling with F-18 through novel reaction chemistry. **T. Ritter**

10:50 – 588. Synthesis, indirect radiolabeling, and bioconjugation studies of [^{18}F]sulfonyl fluoride based synths. **B.H. Fraser***, N.A. Wyatt, B. Zhang, L. Matesic, M.P. Roberts, I. Greguric, T.Q. Pham, A.J. Robinson, G. Pascal

* Principle Author

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Final Pacificchem 2015 program online at:

<http://pacificchem.org/onlineprogram>

11:20 – 589. Aluminum fluoride chemistry: From bench to bedside translation.
X. Chen*

Royal Hawaiian
Regency II

Cancer-Targeted Delivery of Therapeutics and Diagnostics (#393)

Organized by: Y. Kwon, K. Kaur, W. Kim,
Y. Shen
Presiding: Y. Kwon

8:00 – 590. Peptide-functionalized microcantilever arrays as detection platforms for circulating tumor cells in human blood.
K. Kaur, H. Etayash, T. Thundat

8:30 – 591. Selective inhibitors of glutathione transferase P1 with 1,2,4-trioxane structure as anticancer agents.
M.L. Bräutigam, A.G. Griesbeck, M. Pietsch, N. Teusch

8:50 – 592. Diagnostic and therapeutic targeting of EGF-receptor positive cancer cells using single-domain antibodies.
K. Zarschler*

9:20 – 593. Structural control and visualization of a smart bispecific and variable antibody.
H. Fujii, Y. Tanaka, H. Nakazawa, R. Asano, I. Kumagai, M. Umetsu*

4:45 Break

9:50 – 594. Bubble-generating carrier systems for localized controlled release.
K. Chen, M. Chung, C. Hsiao, Z. Liao, W. Chia, K. Lin, **H. Sung***

10:20 – 595. Enhancement of EPR effect of nanomedicine by using nitric oxide-releasing liposome.
T. Yoshikawa*, Y. Tahara, A. Kishimura, T. Mori, Y. Katayama

10:45 – 596. Development of a dual pH- and thermo-responsive magnetic nanocarrier for application in thermo-chemotherapy of cancer.
A. Hervault*, A. Dunn, M. Lim, T. Yoshiaki, K. Matsumura, D. Mott, S. Maenosono, T.T. Nguyen

11:10 – 597. Targeted nanomedicine for cancer therapy.
A. Lavanifar*, K. Kaur, S.M. Garg, R. Soudy

Saturday Afternoon

Sheraton Waikiki
Maui

Academic Drug Discovery (#69)

Organized by: J. Leahy, A. Mendonca, S. Hong, H. Kakeya, P. Scammells
Presiding: J. Leahy

13:00 – 598. Synthesis of potential chaperone inhibitors as novel antileishmaniasis agents.
J. Leahy*, D.E. Kyle

13:20 – 599. Dual inhibition of *Plasmodium falciparum* M1 and M17 metalloaminopeptidases by a novel series of hydroxamic acid-based Inhibitors.
P.J. Scammells*, S. McGowan, N. Vinh, N. Drinkwater

13:40 – 600. Medical structural genomics of pathogenic protozoa and its follow-up drug discovery efforts for protozoan infections.
E. Fan*, C. Verlinde, E. Merritt, W. Van Voorhis, F.S. Buckner, W.G. Hol
14:00 – 601. Neglected tropical disease drug discovery using a distributed drug discovery model.
M.P. Pollastrini*

14:30 – 602. Does plasmeprin V make the 'cut' as an antimalarial drug target?
B.E. Sleeb*, T. Hodder, M. Gazdik, C. Peter, P. Rajasekaran, D. Marapana, M. O'Neill, K. Lowes, B. Smith, A. Cowman, J. Boddy

14:50 – 603. Open source approaches to drug synthesis, discovery, and development.
A. Williamson, P. Willis, P. Olliaro, J. Castro-Pichel, J. Baiget, **M. Todd***

15:10 – 604. Discovery of Q203, a novel chemical entity as a drug candidate for the treatment of tuberculosis.
J. Kim*
15:40 – 605. Drug discovery for malaria in the age of multidrug resistance and the malaria eradication campaign.
D.E. Kyle*, R. Manetsch

16:20 – 606. Discovery of novel therapeutics for treating various types of viral diseases, cancers, and inflammatory disorders.
D.C. Liotta*

Sheraton Waikiki
Honolulu

Small Molecule Epigenetic Modulators (#146)

Organized by: C. Burns, P. Brown, S. Frye
Presiding: P.J. Brown, S.V. Frye

13:00 Introduction

13:05 – 607. Targeting epigenetic pathways to treat cancer.
C. Carpenter

13:35 – 608. Novel inhibitors of BET bromodomains.
C. Burns*, P.P. Sharp, J. Garner

14:05 – 609. LP99: Discovery and synthesis of the first selective BRD7/9 bromodomain inhibitor.
P. Clark, L. Viera, C. Tallant, O. Fedorov, D. Singleton, C. Rogers, O. Monteiro, J. Bennett, R. Baronio, S. Muller, D. Daniels, J. Mendez, S. Knapp, P. Brennan*, **D.J. Dixon***

14:35 – 610. Kinetically selective inhibitors of histone deacetylase 2 (HDAC2) as cognition enhancers.
E. Holson*
15:05 Break

15:25 – 611. SGI-110, journey from discovery to phase 3 for a new generation of DNA hypomethylating agents.
M. Azab*

15:55 – 612. Development of DNA methyltransferase inhibitors using computational approaches.
J.L. Medina-Franco, E. Fernández-De-Gortari, J. Naveja, O. Méndez-Lucio, J. Yoo

16:25 – 613. From hit to clinic, the discovery and preclinical development of the EZH2 inhibitor EPZ6438.
R. Chesworth

16:55 Closing Remarks

Sheraton Waikiki
Waianae

In Vivo Chemical Strategies for Functional and Translation Studies of Biological Networks and Pathways (#212)

Organized by: M. Bogyo, K. Kikuchi, B. Cravatt, H. Kwon

13:00 – 614. Chemical biology tools for manipulating β -cell signaling.
C. Schultz*

13:30 – 615. Linking carbohydrate signaling to cancer metabolism and tumor growth.
L. Hsieh-Wilson*

14:00 – 616. Redox imaging with europium.
M.J. Allen*

14:30 – 617. Chemical tools for monitoring and manipulating the immune system.
T. Kodadek*

15:00 – 618. Membrane-permeant sulfonate dyes for live cell imaging.
M. Schultz, R. Müller, C. Schultz*

15:20 – 619. Effect of drug residence time on in vivo drug efficacy.
K. Lee, J. Yang, J. Liu, C.J. Ng, K. Wagner, H. Dong, J. Liu, B. Hammock*

15:40 break

15:50 – 620. Development of MRI and positron emission tomography (PET) probes for noninvasive detection, staging, and measuring response to treatment in fibrotic disorders.
P. Caravan

16:20 – 621. Development of multifunctional ^{19}F MRI contrast agents with fluorine-encapsulated silica nanoparticle.
K. Kikuchi*

Sheraton Waikiki
Lanai

Molecular Design in Medicine: Concept to Commerce (#295)

Organized by: J. Siegel, M. Martinelli, M. Brimble, M. Platz, H. Wong, K. Baldridge
Presiding: H. Wong

13:00 – 622. Chemical adventures in the natural world.
R.P. Borris*

13:25 – 623. Development of silicon-based biological active compounds by focusing on silyl functional as a *cis*-olefin mimetic.
D. Kajita, M. Nakamura, Y. Matsumoto, M. Ishikawa, Y. Hashimoto, S. Fuji*

13:40 – 624. Development of therapeutic agents from a New Zealand perspective.
M.A. Brimble*

14:05 – 625. Syrbactins: New structural class of natural product-inspired protease inhibitors.
A.S. Bachmann*, M. Pirring, C. Archer, J. Opoku-Ansah, M. Grob, R. Dudley

14:30 – 626. Novel bioactive conjugate agents targeting both estrogen receptor and histone deacetylase for treatment of breast cancer.
H. Zhou*

14:45 – 627. Self-assembled synthetic ion channels.
D. Yang*

15:10 – 628. Synthetic analogs of diphosphoinositol polyphosphates (Ins $_P_7$).
H.J. Jessen*

15:35 – 629. Bioactive molecules/scaffolds derived from symbionts.
R.X. Tan*

16:00 – 630. Template creation to the selective functional group introduction-applications in molecular library synthesis for drug discovery.
J. Huang*

16:15 – 631. Seeking opportunities for C–H functionalization methods in organic synthesis.
E.J. Sorenson*

Sheraton Waikiki
Oahu

Non-canonical Approaches to ^{18}F -labeling: New Frontiers in Stable Non-carbon-fluorine Bonds (#337)

Organized by: D. Perrin, F. Gabai, F. Li, R. Schirrmacher

13:00 – 632. High affinity chelators of fluorine-18.
R. Bhalla*, A. Jackson

13:30 – 633. Increasing the specific activity of isotope exchange radiofluorination using microfluidics.
M.S. Lazar, M.E. Sergeev, Z. Liu, D. Perrin, R. van Dam*

14:00 – 634. Zwitterionic boron-based $[^{18}\text{F}]$ -fluoride captors.
K. Chansaenpak, m. wang, s. liu, F.P. Gabai, Z. Li

14:30 – 635. ^{18}F -labeling of large molecules for multimodality imaging applications.
R. Ting

15:00 Break

15:15 – 636. Design and synthesis of boron containing retinoid based potential PET Imaging agent for glioblastoma.
B.C. Das, K.F. Ginn, A. Mintz

15:35 – 637. Cationic boranes and trifluoroborates: Attractive alternate introduction of ^{18}F .
E. GRAS*, D. Pla-Queral, B. Mestre, C. Perrio, S. Schmitt, K. Chansaenpak, F.P. Gabai

16:05 – 638. ^{18}F -boramino acid: The traceable amino acid mimics for cancer imaging.
Z. Liu, X. Chen

16:35 – 639. Development of trifluoroborate-LLP2A peptidomimetic conjugates as VLA-4-specific ^{18}F -radiotracers for in vivo PET imaging of melanoma.
A. Roxin*, S. Huh, K. Lin, F. Benard, D. Perrin

16:50 – 640. Fluorine-18 labeling of biomolecules using silicon-fluoride chemistry.
S.M. Ametamey*

Royal Hawaiian
Regency II

Cancer-Targeted Delivery of Therapeutics and Diagnostics (#393)

Organized by: Y. Kwon, K. Kaur, W. Kim, Y. Shen
Presiding: K. Kaur

13:00 – 641. Polymeric nanoparticles for cancer-targeted drug and gene delivery.
W. Kim*

13:30 – 642. Hemagglutinating virus of Japan envelope as a versatile vector for photodynamic therapy against advanced and recurrent prostate cancer.
M. Inai*, N. Honda, H. Hazama, H. Nakamura, H. Yasuda, T. Nishikawa, Y. Kaneda, K. Awazu

13:55 – 643. Iron oxide nanocubes coated with thermoresponsive polymers for magnetically induced hyperthermia and drug delivery.
D. Niculaes, T. Mai, H. Kakwre, M. Matera, T. Pellegrino*

14:20 Break

14:25 – 644. Harnessing oncolytic adenovirus for tumor targeting by nanocomplex.
C. Yun*

14:55 – 645. Glutathione responsive anti-proliferative nanoparticle for efficient delivery of therapeutic gene in colon cancer xenograft mouse model.
I. Park*, H. Park, S. Lee, I. Kwon

15:20 – 646. Development of boronated liposomes as efficient boron delivery vehicles for neutron capture therapy.
H. Nakamura*, s. Tachikawa, C. Viñas, M. Suzuki, K. Ono

15:45 – 647. Molecular targets: Emerging trends in personalized cancer therapeutics.
S.M. Blah*†

16:10 – 648. Targeted and synergistic therapy for leukemia using viral/nonviral chimeric nanoparticles.
C. Hong, S. Cho, J. Kim, B. Pham, Y. Kwon*

Saturday Evening

Hawaii Convention Center
Halls I, II, III

In Vivo Chemical Strategies for Functional and Translation Studies of Biological Networks and Pathways (#212)

Organized by: M. Bogyo, K. Kikuchi, B. Cravatt, H. Kwon

Poster Session

19:00 – 21:00

649. Metabolomic profiling of kidney-yang deficiency mice model infected with influenza virus and Mahuang-Xixin-Fuzi decoction treatment.
Q. Sun, H. Jiang, L. Gong, Y. Yang, Z. Yang, J. Tian*, R. Rong*

650. Stable isotope resolved metabolomics (SIRM) of fresh human tissue slices as a preclinical drug testing platform.
T.W. Fan*, A. Belshoff, J. Tan, M. Bousamra, J.T. Martin, R.M. Higashi, A.N. Lane

651. Understanding photosensitization caused by ingestion of the pasture legume *Biserrula pelecinus*.
J.C. Quinn*, S. Gurusinghe, X. Zhu, L.A. Weston

652. New caging agent having a PNA tag for sequence selective nucleotide caging.
W. Hashiba, T. Furuta*

653. Chemo-enzymatic preparation of site-selectively modified caged DNAs.
S. Tada, W. Hashiba, E. Ikeda, A.Z. Suzuki, T. Furuta*

654. Design and synthesis of clickable caged compounds.
A.Z. Suzuki, R. Aikawa, K. Kakehi, T. Furuta*

655. Stimulus-responsive antimicrobial peptides for compound release from nanocarrier.
M. Kashibe, S. Mizukami, K. Kikuchi

656. Two-photon live imaging of osteoclastic bone resorption in living mice using pH-activatable fluorescence probe.
H. Maeda*, T. Kowada, K. Kikuchi

657. Improvement of photostability of fluorescent dyes by using lanthanide complex.
T. Imoto, S. Mizukami, K. Kikuchi

* Principle Author

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658. Development of activatable ^{19}F MRI contrast agents based on paramagnetic relaxation enhancement. **K. Akazawa***, F. Sugihara, Y. Yoshioka, S. Mizukami, K. Kikuchi

659. Development of detection system for histone deacetylase activity using fluorescent probe and DNA. **M. Minoshima**, T. Matsumoto, K. Kikuchi*

660. Development of fluorescent probe for visualizing local Mg^{2+} dynamics in living cells. **Y. Matsui**, S. Mizukami, Y. Funato, H. Miki, K. Kikuchi

Hawaii Convention Center
Halls I, II, III

Molecular Design in Medicine: Concept to Commerce (#295)

Organized by: J. Siegel, M. Martinelli, M. Brimble, M. Platz, H. Wong, K. Baldridge

Poster Session 19:00 – 21:00

661. Design and synthesis of novel ROR inverse agonists based on silicon-containing heterocyclic core structure.

H. Toyama, M. Nakamura, Y. Hashimoto, S. Fuji*

662. Quantitative prediction of kinase inhibitor selectivity. **X. Wen***, H.T. Li*, Y. He, Q. Yu, Z. Xi*

663. Studies on structural modification of gossypol and its antitumor activity.
H. Chen*

Hawaii Convention Center
Halls I, II, III

Cancer-Targeted Delivery of Therapeutics and Diagnostics (#393)

Organized by: Y. Kwon, K. Kaur, W. Kim, Y. Shen

Poster Session 19:00 – 21:00

664. Oxygen releasing hollow microparticles for prolonged cell survival in hypoxia. **H. Lee, H. Kim, J. Lee, S. Oh***

665. Synthesis and functional evaluation of doxorubicin-loaded and gelatin-modified Gd_2O_3 nanoparticles (DOX-gelatin- Gd_2O_3 nanoparticles) as a theranostic probe. **Y. Imai***, Y. Kimura, H. Imai, T. Matsuda, A. Toshimitsu, T. Kondo

666. Design, synthesis, and evaluation of tamoxifen derivatives as new selective estrogen receptor down-regulators. **T. Shoda***, M. Kato, K. Okuhira, Y. Demizu, H. Inoue, M. Naito, M. Kurihara

667. Enhanced transduction efficiency and antitumor efficacy of oncolytic adenovirus coated with bioreducible polymer in the treatment of CAR-negative tumors. **S. Jung, S. Lee**, D. Kasala, J. Choi, S. Kim, C. Yun*

668. Design and biological evaluation of cell-penetrating peptide-curdurumin conjugates as prodrugs. **A. Nasrolah Shirazi**, N.s. El-Sayed, R.K. Tiwari, K. Parang*

669. Photosensitizer-trastuzumab conjugates for targeted photodynamic therapy in a gastric cancer model. B. Korsak, C. Oliveira, B. Sarmento, J.P. Tomé, R.J. Schneider*

670. Development of photoreactive silicon wafer and magnetic beads for isolating target cells based on photolysis of 8-quinolonyl sulfonate based linkers. **K. Matsumoto**, R. Takeda, S. Ariyasu, Y. Mukai, S. Aoki

671. Design and synthesis of PEGylated hydroxamic acid-type histone deacetylase inhibitor prodrugs having targeting ability to cancer tissues. **G. Kimura**, H. Aihara, H. Kamijo, M. Katsuragi, Y. Fukushima, S. Uesato, T. Sumiyoshi, Y. Nagaoka*

Sunday Morning

Sheraton Waikiki
Maui

Academic Drug Discovery (#69)

Organized by: J. Leahy, A. Mendonca, S. Hong, H. Kakeya, P. Scammells
Presiding: P.J. Scammells

8:00 – 672. Vanderbilt Center for Neuroscience Drug Discovery. **C.W. Lindsley**

8:40 – 673. Effort to develop a pre-emptive treatment of Alzheimer disease targeting $\text{GA}\beta$. **A. Kawai***, K. Yanagisawa*, K. Takahashi, T. Hiramoto, M. Kawanishi

9:00 – 674. Structure based design of covalent Inhibitors of LRRK2 kinase mutants linked to familial Parkinson's disease. **S. Ray***, M. Liu*

9:20 – 675. Uncovering potential of Indonesian medicinal plants for dual actions as anti-diabetes and anti-obesity. **L. Lahrita***, E. Kato, J. Kawabata

9:40 – 676. Harnessing nature's biodiversity for therapeutics. M. Apaya, L. Acuram, C.C. Hernandez*

10:00 – 677. Drug discovery based on microbial bioactive natural products. **T. Sunazuka***, S. Omura

10:40 – 678. Stiologlycobiology and targeting disease processes. **M. von Itzstein**

11:20 – 679. Seeking the right TRAIL: reassignment of a cancer therapeutic that has advanced to clinical trials. **K.D. Janda***

Sheraton Waikiki
Honolulu

Small Molecule Epigenetic Modulators (#146)

Organized by: C. Burns, P. Brown, S. Frye

Presiding: C. Burns

8:00 Introduction

8:05 – 680. Targeting histone lysine methylation in cancer. **P. Trojer***

8:35 – 681. Progress toward chemical probes for methyl-lysine readers. **S.V. Frye***

9:05 – 682. Epigenetic chemical probes for target validation. **P.J. Brown***

9:35 Break

9:50 – 683. Targeting epigenetic modifiers:

Potent selective inhibitors of protein arginine methyltransferase 5. **I. Street***, H. Falk, Y. Bergman, S. Walker, S. Sonderegger, E. Allan, J. Baell, M. Camerino, L. Cerruti, S. Charman, M. de Silva, M. Devlin, O. Dolozal, R. Fotzik, D. Ganame, J. Grusovin, S. Hermans, C. Hemley, I. Holmes, W. Kersten, H. Lagiakos, R. Lessene, K. Lowes, G. Lunniss, B. Morrow, A. Natoli, M. Parker, T.S. Peat, J. Pinson, P. Pilling, S. Spall, A. Stupple, Y. Tan, A. Thistlethwaite, E. Toumlin, K. White, D. Curtis, S. Jane, B. Monahan, P. Stupple*

10:20 – 684. Design of peptidomimetics and non-peptide small-molecule inhibitors to target the MLL-WDR5 protein-protein interaction. **S. Wang***

10:50 – 685. Generation of chemical similarity models as filters for virtual screening of LSD1 reversible allosteric inhibitors. **G.L. Genesi**, V.G. Maltarollo, G.H. Troissini*

11:20 Closing remarks

Sheraton Waikiki
Waianae

In Vivo Chemical Strategies for Functional and Translation Studies of Biological Networks and Pathways (#212)

Organized by: M. Bogyo, K. Kikuchi, B. Cravatt, H. Kwon

8:00 – 686. Development of protein-tag-based research tools in live cell imaging. **S. Mizukami***, K. Kikuchi

8:20 – 687. Modular caging groups – new platforms for multifunctional caged compounds. **T. Furuta**

8:50 – 688. Identification of small molecule modulators of cancer stem cells via phenotype-specific cell binding screening with combinatorial chemical library. **L. Chen, C. Long, J. Lee***

9:20 – 689. Exploiting exogenous chemistry for intracellular protein manipulations. **P. Chen***

9:50 – 690. Reverse chemical proteomics with natural products for cellular and clinical applications. **P. Karuso***, A. Piggott, M. Gotsbacher

10:20 break

10:30 – 691. Emerging approaches and challenging targets in drug discovery. **R. Hannoush**

11:00 – 692. Target identification of bioactive small molecules toward functional and translational studies of angiogenesis. **H. Kwon***

Sheraton Waikiki
Lanai

Molecular Design in Medicine: Concept to Commerce (#295)

Organized by: J. Siegel, M. Martinelli, M. Brimble, M. Platz, H. Wong, K. Baldridge

Presiding: M. Martinelli

8:00 Speaker Prep

8:30 – 693. Timely chemical process research is a critical part for efficient drug development. **C. Senanayake**

8:55 – 694. Route design toward durable simplicity. **T.Y. Zhang**

9:20 – 695. Discovery of MK-8449, a SYK/ZAP70 inhibitor for rheumatoid arthritis. **A. Haidele***, M. Altman, K. Childers, M. Ellis, C. Fischer, F. Gervais, H. Houshyar, S. Kattar, S. Lee, M. Lowinger, M. Maddess, R. Miller, A. Northrup, R. Otto, A. Schell, S. Vincent

9:35 – 696. Biological roles of sterol glycosides within the context of an integrated chemical ecology. **J. Gervay Hague***

10:00 – 697. Process development of drug candidates post approval: A case study for a Gamma amino acid candidate. **T. Braish***

10:25 – 698. Aging, neurodegeneration, and chemical targeting of mitochondria. **P. Wipf***

10:50 – 699. Discovery and optimization of a novel series of LPA receptor antagonists with efficacy in multiple mouse models of fibrosis. **J. Seiders**

11:15 – 700. Developing an international pharmacy school in Tianjin, China. **J. Siegel**

Royal Hawaiian
Regency II

Cancer-Targeted Delivery of Therapeutics and Diagnostics (#393)

Organized by: Y. Kwon, K. Kaur, W. Kim, Y. Shen

Presiding: W. Kim

8:00 – 701. Anticancer nanomedicines through controlled chemistry. **J. Cheng***

8:30 – 702. Multifunctional liposomes having target-specificity, imaging, and temperature-responsive drug release for cancer chemotherapy. **K. Kono***, M. Takashima, E. Yuba, A. Harada, D. Kokuryo, I. Aoki, K. Maruyama, S. Aoshima

8:55 – 703. High throughput screening of cancer therapeutic small antibody designed from domain library. **A. Sugiyama**, M. Umetsu, H. Nakazawa, K. Hosokawa, R. Asano, I. Kumagai

9:20 – 704. On-chip profiling of clinically relevant exosomes using a SPR biosensor. **L.G. Carrascosa**, A. Sina, R. Vaidyanathan, S. Dey, M. Shiddiky, M. Trau

9:45 Break

9:50 – 705. New strategies for imaging infectious diseases and oxidative stress. **N. Murthy***

10:20 – 706. "Caged" molecular glue uncaged by cancer specific signal. **C. Chen**, J. Hatano, K. Okuro, T. Aida

10:45 – 707. Dendrimer porphyrin-incorporated nanoparticles for cancer theragnosis. **W. Koh***, U. Chung

11:10 – 708. Development of mixed nano-structure composed of self-assembled monolayer and ultrathin silver chloride for electrochemical biosensing. **M. TABATA**, T. Goda, A. Matsumoto, Y. Miyahara*

11:35 – 709. Radioembolization with second generation biodegradable microspheres. **K. SAATCHI**, M. Bokharaie, A. Thakor , P. Esquinias, J. De La Vega, A. Celler, D. Liu, U. Hafeli

SCTY

Area 11 – Connecting Chemistry to Society

Tuesday Morning

Hawaii Convention Center
303A

The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other and with Society (#173)

Organized by: J. MacLachlan, A. Williams, K. Hayashi, D. Martinsen, B. Brown
Presiding: J. MacLachlan

8:00 Opening Remarks

8:05 – 1. Social media and *Inorganic Chemistry*: Successes and challenges. **W.B. Tolman***

8:45 – 2. Chem-Station: A virtual location where chemists assemble. **J. Yamaguchi**

9:10 – 3. Digital tools for the chemist: An editor's perspective. **G. Armstrong***, S. Cantrell, S. Davey, A. Pichon, R. Johnson

9:50 – 4. The social author, the social publisher. **E.C. Wiring***

10:15 – 5. Turning the tide: The "article last" content approach. **A. Brownsell**

10:55 – 6. A Christmas Carol: The evolving landscape of scientific publishing. **J.Y. Chen***, D. Martinsen

11:20 – 7. Opportunities for chemists to have meaningful interactions and do better science through social media platforms. **W. Dichtel**

Hawaii Convention Center
302A

Bioactive Natural Products and Public Health in the Pacific Rim: From Aquatic Dietary Supplements to Marine and Freshwater Toxins (#230)

Organized by: J. Hungerford, W. Rourke, P. McNabb, J. Betz
Presiding: J.M. Betz

8:00 Joseph Betz

8:05 – 8. Exploring for bioactive secondary metabolites from Chinese medicinal mangroves. **Y. Guo***

* Principle Author

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organizers and individual presenters.

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8:45 – 9. Identification of marker compounds to distinguish herbal medicines originating from different *Vitex* species.
S. Masada, N. Oshima, T. Yahagi, R. Suzuki, Y. Takahashi, H. Matsufuji, M. Watanabe, S. Yahara, O. Iida, N. Kawahara, T. Maruyama, Y. Goda, **T. Hakamatsuka***

9:05 Break
9:20 – 10. Nuclear magnetic resonance-based metabolomics of hawthorn species for natural health product optimization. J.A. Lund, P.N. Brown, **P.R. Shipley***
9:40 – 11. Cyanobacteria reference materials: Design and development. **C.A. Rimmer**, A. Stindt, L. Sander
10:20 – 12. Cyanobacteria in the dietary supplement and natural health product marketplace. **J.M. Betz***

Hawaii Convention Center
302B

Chemistry Education: International and Multicultural Perspectives (#365)

Organized by: S. Sandi-Urena, D. Salter, C. Do
Presiding: C.H. Do, C.V. Gauthier

8:00 Introductory remarks
8:05 – 13. Development of microscale corrosion experimental teaching materials for engineers. **D. Ito***
8:25 – 14. First chemistry and biology joint laboratory course in English for international students at the University of Tokyo. **Y. Nakamura***, M. Wang, M. Sato
8:45 Intermission
9:00 – 15. Establishing successful interdisciplinary collaborations in Peru. **C. V. Gauthier***
9:20 – 16. PROJECT SEED: Summer research experiences for economically disadvantaged high school students. **A.G. Cavinato*, C. Hernandez**
9:40 – 17. Reach-out and pro bono programs for the dissemination of chemical knowledge. **C.H. Do***
10:00 Discussion

Hawaii Convention Center
303B

Safety in the Academic Research Laboratory (#460)

Organized by: E. Reichmanis, H. Horton, D. Kennedy

8:00 Elsa Reichmanis
8:05 – 18. Safe science: Promoting a culture of safety in academic research. **H. Thorp***
8:35 – 19. Safety first culture in Australian laboratories. **A. Vecchio-Sadus***
9:05 – 20. Comprehensive and effective program for environmental safety education in universities. **Y. Tsuji***
9:35 – 21. Laboratory safety in ChBE at Georgia Tech and the PALS collaboration with ExxonMobil. D. Sholl, **S. Nair**, C. Dixon, T. Alford
10:05 – 22. International differences in laboratory safety preparation for chemistry graduate students. **R. Phifer**
10:25 – 23. Evolution of safety culture in University of California academic research laboratories. **J.G. Palmer, L. Wong***
10:45 – 24. Laboratory scale risk assessment. **N. Langerman**
11:05 – 25. Study of students' engagement in various styles of safety videos. **H. Weizman***

Tuesday Afternoon

Hawaii Convention Center
303A

The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other and with Society (#173)

Organized by: J. MacLachlan, A. Williams, K. Hayashi, D. Martinsen, B. Brown
Presiding: J. MacLachlan

13:00 Opening Remarks
13:05 – 26. Don't panic: A scientist's guide to Twitter. **K.E. James***
14:05 – 27. Engaging students, alumni, and colleagues through social media. **S.C. Burdette**
14:35 – 28. Reactions to the open spectral database. **S.J. Chalk**
15:05 – 29. Open science framework (osf): A free, open source platform for sharing research works. **S.D. Bowman**
15:30 – 30. Open software platforms for chemistry on the desktop and web. **M. Hanwell***
15:55 – 31. Implementing and assessing the efficacy of open access chemwiki textbook resource. **D.S. Larsen***
16:20 – 32. Is Twitter changing the face of science?. **B. Campos Seijo***

Hawaii Convention Center
302A

Bioactive Natural Products and Public Health in the Pacific Rim: From Aquatic Dietary Supplements to Marine and Freshwater Toxins (#230)

Organized by: J. Hungerford, W. Rourke, P. McNabb, J. Betz
Presiding: J. Hungerford

13:00 James Hungerford
13:05 – 33. Analytical methods and reference materials for cyanobacterial toxins. **M.A. Quilliam**, D. Beach, P. McCarron, C. Hollingdale, E. Kerrin, K. Thomas, S. Giddings, N. Lewis
13:45 – 34. Natural environmental neurotoxins: The case of β -N-methylamino-L-alanine. **S. Murch***
14:20 – 35. Accurate detection and quantification of β -N-methylamino-L-alanine in food and environmental samples. **T.C. Baker***, S. Murch, **P.N. Brown**

14:55 Break
15:10 – 36. Screening assays for new polytoxin analogs detection. **A. Tubaro***, M. Pelin
15:40 – 37. Marine STAR: Getting environmental contaminant data to the masses. **J.M. Ragland***, J.L. Reiner, S.S. Vander Pol, R. Pugh, P. Becker
16:00 – 38. In the Pacific Rim with AOAC's Marine and Freshwater Toxins Task Force. **J. Hungerford***

Hawaii Convention Center
302B

Chemistry Education: International and Multicultural Perspectives (#365)

Organized by: S. Sandi-Urena, D. Salter, C. Do
Presiding: C.H. Do, C.V. Gauthier

13:00 Introductory remarks
13:05 – 39. Teaching methodologies for how to fully integrate students who are blind into chemistry laboratory experiences. **C.A. Supalo***
13:25 – 40. Identity, intersectionality, and the culture of science. **M. Grunert Kowalske***
13:45 – 41. Educating LGBT chemical scientists: Mentoring, professional associations, and successful integration of the whole person. **C.J. Bannonie***, B. Belmont, R. Hernandez
14:05 – 42. Bringing "relevance" into the chemistry curriculum. **G.M. Bodner***
14:35 Intermission
14:50 – 43. Demarginalizing global competency and global citizenship in the 21st century chemistry classroom: The risks and benefits of a deprogrammed chemistry program. **J. Bhattacharya***
15:10 – 44. Trends, opportunities, and best practices in graduate chemistry study abroad. **R. McKimmon***, B. Miller

15:30 – 45. Global Chemists Code of Ethics: How international collaboration can lead to sustainable, responsible chemistry education. **S. Hill***, J. Uddin Ahmad*, B. Miller
16:00 Discussion

Hawaii Convention Center
303B

Safety in the Academic Research Laboratory (#460)

Organized by: E. Reichmanis, H. Horton, D. Kennedy

13:00 – 46. From accident analysis to accident prevention at UCLA. **C. Merlic***, I. Schroeder

13:20 – 47. A student's perspective on safety in the academic lab. **N. Persson***, E. Reichmanis

13:40 – 48. Assessment and management of chemical risks in academic laboratories

(1) Important factors for risk assessment in chemical laboratories. **H. Yamamoto***, Y. Nezu, Y. Oshima

14:00 – 49. Advancing safety culture in academic research laboratories: A case study. **L.M. Gibbs***

14:20 – 50. Assessment and management of chemical risks in academic laboratories

(2) Influence of laboratory layout on airflow in university laboratory. **Y. Nezu***, Y. Nabeshima, H. Yamamoto, Y. Oshima

14:40 – 51. Assessment and management of chemical risks in academic laboratories

(3) Observing behavior of experimenter and chemical reagents in an actual chemical laboratory. **Y. Oshima***, Y. Nezu, H. Yamamoto

15:00 – 52. Ensuring a safe and successful research laboratory for deaf and hard-of-hearing undergraduate students. **T. Pagano***, A.D. Ross, S.B. Smith

15:20 – 53. Supporting a prudent safety culture through job hazard analysis and information literacy skills. **R.B. Stuart**

15:40 – 54. Critical role of public access to

chemical data and information in supporting safety culture in academic research laboratories. **L. McEwen**, E. Bolton, S. Heller

16:00 – 55. Leveraging academic safety culture as a value-added tool for maximizing the undergraduate research experience. **G.M. Ferrence***, N.K. Fredstrom

Wednesday Morning

Hawaii Convention Center
303A

The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other and with Society (#173)

Organized by: J. MacLachlan, A. Williams, K. Hayashi, D. Martinsen, B. Brown
Presiding: J. MacLachlan

8:00 Opening Remarks by Tom Connelly, Executive Director and CEO of the American Chemical Society

8:05 – 56. Linked-In® and Facebook® for business: Learn how to leverage these powerful social tools. **J. MacLachlan**

8:30 – 57. Connecting through social media (Part I). **M. Feliu-Mojer***, R.M. Burks, L. Neeley, D. Lee, B. Lillie

9:00 – 58. Connecting through social media (Part II). **M. Feliu-Mojer***, R.M. Burks, L. Neeley, D. Lee, B. Lillie

9:30 – 59. Connecting with the media (Part I). **R.M. Burks***, L. Neeley, M. Feliu-Mojer, D. Lee, B. Lillie

10:00 – 60. Connecting with the media (Part II). **R.M. Burks***, L. Neeley, M. Feliu-Mojer, D. Lee, B. Lillie

10:30 – 61. Reaching your target audience after publication. **L. Stemmler***

11:00 – 62. Scholarly journals in China involved in Friends circles: Promotion or profit. **X. Zhu**

11:30 – 63. ACS Crystal Growth & Design: Founding a journal in the cusp of electronic publishing and open access. **R.D. Rogers**

Hawaii Convention Center
Halls I, II, III

Bioactive Natural Products and Public Health in the Pacific Rim: From Aquatic Dietary Supplements to Marine and Freshwater Toxins (#230)

Organized by: J. Hungerford, W. Rourke, P. McNabb, J. Betz

Poster Session

10:00 – 12:00

64. Anti breast cancer effect of *Ecklonia* caava-derived dieckol. **N. Jeon**, Y. Kim, J. Hwang, S. Kim, B. You, X. Dong

Hawaii Convention Center
302B

Chemistry Education: International and Multicultural Perspectives (#365)

Organized by: S. Sandi-Urena, D. Salter, C. Do
Presiding: C.H. Do, I. Montes

8:00 Introductory remarks

8:05 – 65. ASClV2 as a tool to investigate student attitudes in Australia and the United States. **J. Alexander***, A.T. Baker, S. Chadwick

8:25 – 66. Sink or swim: Perspectives of tertiary pedagogical content knowledge (PCK). **G.A. Lawrie***, M. Schultz

8:45 – 67. Pedagogical content knowledge in tertiary chemistry: The culture of sub-disciplines. **M. Schultz**, G.A. Lawrie

9:05 – 68. Authentic Thinking with Argumentation (ATA): Learning model for fostering learners could solve problems with scientific thinking and processes. **J. Baek***, D. Jeong

9:25 Intermission

9:35 – 69. Using web-based learning activities to enhance understanding of acids and bases. **S.D. Woodgate***

9:55 – 70. Chemistry education collaborations across cultural and national borders: The Middle East. **M.Z. Hoffman***, Z.M. Lerman

10:25 – 71. "Festival de Química," a successful international non-formal educational model. **I. Montes**

10:55 Discussion and concluding remarks

Hawaii Convention Center
302A

Women in Chemistry: Changing the Face of Science (#382)

Organized by: E. Nalley, K. Kurihara, V. Chen, L. Watkins
Presiding: V. Chen, E. Nalley

8:00 Opening Remarks

8:25 – 72. Women leaders of the Global Chemistry Enterprise. **M. Wu***

8:50 – 73. Why are women underrepresented in science? Evidence for and against 5 common hypotheses. **K.S. McCain***

9:15 – 74. Change in demographics of STEM faculty at research universities over the last decade. **D.J. Nelson***

9:40 – 75. Women in chemistry: An Australian perspective. **K.A. Jolliffe**

10:05 Break

* Principle Author

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10:30 – 76. Promotion of women scientists and engineers in Japan: Achievements and challenges. **K. Kurihara**
10:55 – 77. Challenges and strategies for increasing participation of women and girls in STEM fields. **C. Cruden***
11:20 – 78. Program to accelerate the appointment of women faculty at Kobe University. **Y. SOUMA***

Hawaii Convention Center
303B

University-Industry Collaboration, Regulatory Environments, and Commercialization of Emerging Technology (#453)

Organized by: E. Reichmanis, S. Usselman, H. Slotten, H. Choi

8:00 Steven Usselman
8:05 – 79. Of Kimchi and spectroscopy: Chili powder, free trade, and the boundaries of regulatory science. **B. Park***

8:35 – 80. Catalyst research for polymer electrolyte fuel cells (CaRPE-FC): A perspective of path to marketplace for nanomaterials through a program in Canada. **T. Naveen*, S. Holdcroft**

9:05 – 81. Commercialization of semiconductor nanomaterials research: A study of the US Department of Energy's Solid-state lighting research program. **A.M. Smith***

9:25 – 82. Centralization and collaboration at Energy Frontier Research Centers. **S.Y. Lai*, A.M. Smith, J. Bea-Taylor, R.B. Hill, N. Kleinhenz**

9:45 – 83. Minerals, metals and materials: Understanding the world around us. **J. Cutler*, L. Van Loon, J. Zhou, J. Reid, J. Olson, T. Bond, E. Bergen**

10:05 – 84. Impact of climate on the LCOE for thin film and crystalline photovoltaic technologies. **M. Smith*, J. McGrath, D. Boylu, L. Yates, D. Gordon, M. Flowers, A. Parsekian**

10:25 – 85. Support for innovation in America's technical workforce from the U.S. National Science Foundation's Advanced Technological Education program. **D.R. Brown***

10:45 – 86. Utilization of advanced radiation facilities under research cooperation with academics. **K. Hirota*, K. Shidomi, H. Sawahata**

11:05 – 87. Nanotechnology in Thailand: Adding value to exports, promoting sustainable development. **J. Bea-Taylor**

11:25 – 88. Industry expectations for new hires – safety awareness. **N. Langerman***

Hawaii Convention Center
Halls I, II, III

Safety in the Academic Research Laboratory (#460)

Organized by: E. Reichmanis, H. Horton, D. Kennedy

Poster Session

10:00 – 12:00

89. Introducing general chemistry students to academic safety culture through participatory case study development. **G.M. Ferrence*, S.M. Scheible**

90. Safety regulations and awareness in the academic research laboratory at a community college. **P. Flores Gallardo***

Wednesday Afternoon

Hawaii Convention Center
303A

The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other and with Society (#173)

Organized by: J. MacLachlan, A. Williams, K. Hayashi, D. Martinsen, B. Brown
 Presiding: J. MacLachlan

13:00 Opening Remarks
13:05 – 91. Advancing chemistry and communicating chemistry for the benefit of Earth and its people. **B.Z. Shakhshiri***

14:05 – 92. Social media and outreach from a National Laboratory perspective. **G.B. Balazs**

14:30 – 93. From the Cape Cod Science Cafe 2011 to STEM Journey 2016: How we have sustained our chemistry outreach beyond the International Year of Chemistry. **J. MacLachlan*, J. Driscoll**

14:55 – 94. Recent progress and future plan of our activities bridging science and society in Japan. **K. Shimada*, M.O. Watanabe, S. Ohtake***

15:20 – 95. Creatively connecting chemistry to society. **G.S. Ruskin***

15:45 – 96. Challenge for scientists of parsing personal vs. organizational social media obligations and observations. **T. Holme**

16:10 – 97. Ethics in publishing: Editorial and related experiences. **P.S. Weiss***

16:35 – 98. Tweeting and cheating – connecting with students as an author. **S. Keam***

Hawaii Convention Center
302B

Effective Collaboration Strategies to Drive Innovation in Drug Discovery and Development (#179)

Organized by: M. Armstrong, S. Kim, Y. Zhu, J. Blount
 Presiding: M. Armstrong

13:00 Opening Remarks

13:05 – 99. How to effectively protect your invention with collaborative research. **M. Armstrong***

13:35 – 100. Tips for choosing and protecting proprietary names and trademarks for drugs. **R.J. Kenney**

14:05 – 101. What early-stage life science companies need to know now: Challenges and opportunities when communicating with the U.S. Food and Drug Administration. **A.G. Minsk***

14:35 Break

14:45 – 102. Successful industry-academia collaboration toward the development of new host-based antivirals against influenza. **E. Marsault, P. Boudreault, M. Azzi, A. Griffin, B. Brown, R. Leduc, M. Richter**

15:15 – 103. Open source pharmaceutical industry. **M. Todd***

15:45 General Questions

15:55 Closing Remarks

Hawaii Convention Center
302A

Women in Chemistry: Changing the Face of Science (#382)

Organized by: E. Nalley, K. Kurihara, V. Chen, L. Watkins
 Presiding: E. Nalley

13:00 Opening Remarks

13:05 – 104. Activities of Gender Equality Promotion Committee in The Society of Chemical Engineering, Japan. **N. Shibasaki-Kitakawa**

13:30 – 105. Women in chemical engineering: Australian perspective. **V. Chen***

13:55 – 106. Encouragement of female students in high school and junior high school to study science. **Y. Hosokoshi*, K. Morizawa, M. Onda, N. Ohmido, S. Kasahara, S. Tajima, M. Shinohara, Y. Matsuoka, T. Kobayashi, T. Tsunemi, Y. Harada, E. Enoki, Y. SOUMA**

14:20 – 107. Gender inequalities: Will the change from past to present stand the test for significance in change? **I. Black**

14:45 Break

15:00 – 108. Transforming the pipette of progress: Growth and opportunities. **A. Wilson**

15:25 – 109. Overcoming the stereotype of the Big Bang theory. **E. Nalley***

15:50 – 110. Positive action for female researchers at Hokkaido University. **M. Kato***

Wednesday Evening

Hawaii Convention Center
Halls I, II, III

The Evolving Nature of Scholarly Communication: Connecting Scholars with Each Other and with Society (#173)

Organized by: J. MacLachlan, A. Williams, K. Hayashi, D. Martinsen, B. Brown
 Presiding: J. MacLachlan

Poster Session

19:00 – 21:00

111. Social media and managing business relationships: Transitioning from marketing to sales of scientific instrumentation. **J. MacLachlan*, J. Driscoll**

112. Visualization of chemistry: Role of graphic design in chemistry. **A. Sato***

113. Connecting the judiciary with science: The legal and social issue of marijuana. **M.A. Celeste**

Hawaii Convention Center
Halls I, II, III

Chemistry Education: International and Multicultural Perspectives (#365)

Organized by: S. Sandi-Urena, D. Salter, C. Do
 Presiding: C.H. Do, S. Sandi-Urena

Poster Session

19:00 – 21:00

114. Learning inquiries for Spanish-speaking exchange students taking chemistry classes at a community college. **G. Coronado*, P. Flores Gallardo***

115. Educational activities within the European Union's Tempus NETREL project. **I. Spanik*, G. Mills, B. Vrana**

116. Development of a pre-service and in-service "Color Science" training program for teachers, in cooperation with Toho University, JACI, and DIC Co., Ltd. **I. Imai*, M. Takahashi, K. Tominaga, K. Makide**

117. From STEM to STEAM: Thermodynamics and the art of Japanese swordsmithing. **C.B. Johnson*, M.M. Day, L. Pesterfield**

118. Research on chemistry education referring to common materials: The effect of UV cosmetics. **M. Karayama, A. AKIMOTO***

119. Application of tablet devices to chemistry classes at college of technology. **H. SATO*, K. Fukumoto, A. OSHIO, Y. HATTORI, O. KATAYAMA**

120. Oxidation reaction experiment of iron powder (disposable warmer) using hand-made oxygen sensor. **M. TAKAHASHI*, Y. Tateizumi**

121. Science craft for chemistry education. **A. Yanase, M. Kamata**

Thursday Morning

Hawaii Convention Center
303A

Green and Sustainable Chemistry Education for Tomorrow's Citizens of the World (#334)

Organized by: J. Jackson, F. Zheng, R. Resendes, D. Kovacs, J. Jackson, K. Saito
 Presiding: J. Jackson

8:00 – 122. Green chemistry programs at the University of Massachusetts Boston. **W. Zhang***

8:25 – 123. Green chemistry education roadmap to advance greener solutions throughout the chemical enterprise. **J. Hutchison***

8:50 – 124. Designing partnerships that drive innovation in general education chemistry courses: Paving the way for a green chemistry education roadmap. **J.A. Haack***

9:15 – 125. Designing effective curricula and assessments to promote deep learning of green chemistry. **M.M. Cooper**

9:40 – 126. Greening the organic lab: A comparison of microwave-assisted and classical nucleophilic aromatic substitution reactions. **D.R. Latimer**

10:00 Break

10:10 – 127. Self-education in green chemistry and engineering – a retrospective look. **D.C. Constable**

10:40 – 128. Greening the curriculum through the School of Green Chemistry and Engineering at the University of Toledo. **G. Lipscomb, M. Mason**

11:00 – 129. Chemistry in engineering education: A course outline for sustainable bioenergy systems. **C.M. Saffron*, F. Pan**

11:20 – 130. Climate change effects and the sustainability of cacao and chocolate. **H.M. Peters*, S.B. Peters**

Hawaii Convention Center
302B

Policies and Procedures Regarding Primary Research Data (#335)

Organized by: D. Martinsen, K. Hayashi, N. Adams

8:00 – 131. What's a publisher to do about research data?. **D. Martinsen***

8:20 – 132. Sharing science data: Semantically reimagining the IUPAC solubility series data. **S.J. Chalk*, R.J. Hanisch, A. Morey, D.R. Burgess, A.Y. Lee**

8:45 – 133. Open science in Japan: Recent progress in policy and research programs. **S. Ohtake*, Y. Ogasaka**

9:15 – 134. A chemical view on research data: Identifying critical structures for management in the machine era. **L. McEwen**

9:45 Break

9:55 – 135. Recent state of policy development and research activities in Japan for sharing research outputs. **K. Hayashi**

10:20 – 136. Helping the chemical science community preserve and share data: An international society publisher's perspective. **J. Griffiths*, D. Zhang**

10:45 – 137. Facilitating and incentivizing openness to enhance reproducibility. **S.D. Bowman**

11:15 – 138. Sustaining access to research data: A 50 year case study. **I. Bruno*, C. Groom**

11:45 Panel Discussion

Hawaii Convention Center
302A

Women in Chemistry: Changing the Face of Science (#382)

Organized by: E. Nalley, K. Kurihara, V. Chen, L. Watkins

Presiding: K. Kurihara

8:00 Opening remarks

8:05 – 139. Tennessee women in chemistry: Changing the face of science. **J. Irarate-Gross***

8:30 – 140. Studying the persistency of women in the field of chemistry in North Carolina. **E.C. Gravely, G.P. Redd**

8:55 – 141. Changing the face of Hiroshima University. **M. Aida***

9:20 – 142. Women in chemistry - a view from the other side. **K. Vitense***

9:45 Break

* Principle Author

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<http://pacificchem.org/onlineprogram>

10:00 – 143. Balancing the equation: A mentoring program for first year female students. **E.J. Smith**, K. Harris, N. Iamsuk, T. McGuren, J. Miller, J. Wilkes, J. Reid
10:25 – 144. Contributions of women chemists toward peace in the Middle East. **Z.M. Lerman***

10:50 – 145. Leadership across multiple cultures: Providing workplace fairness regarding common issues faced by women in chemistry. **K.M. Elkins**, **S.M. Schelble***

11:15 – 146. Positive and sustainable action for gender equality at Nara Women's University. **T. Takeuchi***

Hawaii Convention Center
 303B

Active and Inquiry Learning in the Chemistry Classroom and Laboratory (#443)

Organized by: M. Buntine, S. Boniface, J. Lewis
Presiding: S. Boniface

8:00 Welcome Remarks

8:05 – 147. Process oriented guided inquiry learning (POGL): A student-centered approach to chemistry instruction. **R. Moog***

8:40 – 148. Overview of peer-led team learning (PLTL). **P. Varma-Nelson***

8:55 – 149. Connecting with our students through interactive lecture demonstrations. **S. Schmid***, A. Bridgeman, K.A. Badiola

9:10 – 150. Teaching ethics and professionalism through active learning and engagement. **S.M. Schelble***, **M.C. Loui**, **G.M. Ferrence**

9:25 – 151. Inquiry-driven organic laboratory incorporating current research. A.R. Prosser, D.C. Liotta, **M.F. McCormick***

9:40 – 152. Introducing students to research in second year analytical chemistry laboratories using inquiry-based projects. **J.R. Rodriguez Nunez***, E.J. Maxwell

9:55 Break

10:15 – 153. Improving student engagement in active learning by strengthening self-confidence in the application of underpinning core concepts in chemistry. **V.G. Barnett***

10:30 – 154. Enhancing active learning and student engagement in first year chemistry classes. **E. New***, A. Bridgeman, A. George, P. Rutledge

10:45 – 155. Prion disease as a short, in-lecture, “choose-your-own-experiment” biochemical case to teach nature of science and protein misfolding. **J.K. Hines***, A. Serrano, J. Liebner

11:00 – 156. Active teaching and learning strategies: A synthesis of lecture and lab. **R. Venkateswaran***

11:15 – 157. Experiences with the use of a Classroom Response System (CRS) in a Chemistry Foundation Course. **C.M. Arewgoda***

11:30 – 158. PLTL: A large scale transformative program in general and organic chemistry at UT Dallas. **J. Sibert**

11:45 – 159. Combining green chemistry and guided-inquiry learning to improve students' conceptual understanding. **T.J. Greenbowe**, D. Exton*, B. Baldock

Thursday Afternoon

Hawaii Convention Center
 303A

Green and Sustainable Chemistry Education for Tomorrow's Citizens of the World (#334)

Organized by: J. Jackson, F. Zheng, R. Resendes, D. Kovacs, J. Jackson, K. Saito
Presiding: K. Saito

13:00 – 160. A personal vision of sustainable chemistry at the National Science Foundation. **M.S. Platz***

13:30 – 161. Green chemistry through six editions of *Chemistry in Context*. **C.H. Middlecamp***

13:50 – 162. Making the green chemistry connection with high school students. **D.M. Cullen**

14:10 – 163. Microscale experiment for elementary school science using anthocyanin from grape peel. **T. Nakagawa***

14:30 – 164. Project iLASER: Engaging the public in an appreciation for chemistry with a focus on sustainable energy. **D.R. Brown***

14:50 Break
15:00 – 165. Sustainability and green chemistry: Our role as scientist-citizens. **B.Z. Shakhashiri***

15:40 – 166. Maximizing the impact from an industrial/academic research collaboration: ACS GCI Pharmaceutical Roundtable collaboration with UCLA leads to creation of a new green chemistry teaching lab experiment for undergraduates. **D. Richter***

16:10 – 167. Need for green chemistry at the undergraduate level. **I. Sidhwani**, R. Shama

16:30 – 168. Sustainability benefits of scientific research in the energy industry. **A. Bishop**

Hawaii Convention Center
 302A

Women in Chemistry: Changing the Face of Science (#382)

Organized by: E. Nalley, K. Kurihara, V. Chen, L. Watkins
Presiding: G. Thomas

13:00 Opening Remarks

13:05 – 169. Advancing gender equity at a minority serving institution. **Z.S. Wilson***, G.S. Byrd, S. Luster-Treasley, R. Coger

13:30 – 170. Women chemists of color: An institutional change approach. **K. Mack***, M. Soto, N. Cantor, P. McDermott

13:55 – 171. Ongoing challenges for Hispanic women. **I. Montes***

14:20 Break

14:30 – 172. Progress of women chemists of color in the United States. **G. Thomas**, L.M. Watkins, J. Tiltus-Young, Z.S. Wilson

14:55 – 173. Native American women in STEM. **N. Jackson**

15:20 – 174. A chemical imbalance. P.L. Arnold*, S. Rodnes, M. Liden, C. Conant, **J. Rieb**

Hawaii Convention Center
 303B

Active and Inquiry Learning in the Chemistry Classroom and Laboratory (#443)

Organized by: M. Buntine, S. Boniface, J. Lewis
Presiding: J.E. Lewis

13:00 – 175. Efficacy and cultural transferability of student inquiry learning approaches in foundation chemistry: Improving conceptual understanding and confidence. **S.S. Qureshi***

13:35 – 176. Chemistry in context: Promoting information literacy in the general chemistry lecture and lab. **S. Brydges***

13:50 – 177. Method for the validation of a first year experiment. **R. Pullen**, B.F. Yates, G. Dicinoski, N. Brown, J. Smith

14:05 – 178. Chemistry converged: A pedagogy-led curriculum for the 21st century. **D. Southam***, M. Buntine

14:20 – 179. Evolution and evaluation of a (peer led) team learning implementation in organic chemistry at an undergraduate institution. **J.G. Gillmore***

14:35 – 180. MitoNEET folding and iron sulfur cluster stability investigations in the undergraduate lab course as a unique experiential learning environment. **T.C. Leeper***, D.L. Morris

14:50 – 181. Student perceptions and staff misconceptions about the undergraduate laboratory learning experience. **M. Buntine**, K. Burke da Silva, K.F. Lim, S. Pyke, J. Read, M. Sharma, A. Yeung, S. Kable*

15:05 Break

15:25 – 182. Impact of course preparation assignments on student learning in chemistry and biochemistry courses. **N.J. Ronkainen***

15:40 – 183. Discovery based molecular structure determination lab module integrating chemical crystallography into advanced undergraduate laboratories. **J.M. Tanski***

15:55 – 184. Active learning in chemistry and the transition from high school to university. **S. Boniface***, A. Moed

16:10 – 185. “I’m trying to think of what else we could do”: Analysis of student discourse during pre-lab problem solving sessions. **G.V. Shultz***

16:25 – 186. Using threshold concepts to guide changes in active learning classrooms. **J. Loertscher***, J.E. Lewis, V. Minderhout, T. Morgan, X. Xu

Thursday Evening

Hawaii Convention Center

Halls I, II, III

Green and Sustainable Chemistry Education for Tomorrow's Citizens of the World (#334)

Organized by: J. Jackson, F. Zheng, R. Resendes, D. Kovacs, J. Jackson, K. Saito
Presiding: J. Jackson, F. Zheng

Poster Session

19:00 – 21:00

187. Partnership between university and high schools for wise use of biodiversity. **K. Kanno**, K. Miyagawa, M. Ueno

188. Illustrating green and sustainable chemistry concepts through the synthesis and characterization of renewable triblock copolymer in the organic chemistry laboratory. **J.E. Wissinger**, D. Schneiderman, G. Fahnhorst, M. Wentzel, Z. Swingen

189. Preparation of chiral flavors by asymmetric oxidation. **H. Tian**

190. Teaching of chemistry from green chemistry perspective. **P.J. González***, C. Perez-Mendez, S. Figueroa-Duarte

191. Developing an undergraduate chemistry lab involving mechanochemistry and green chemistry metrics. **S. Kingston**, R. Chetram, T. Hamilton*

192. Green chemistry and sustainability initiatives at the state level: Education through public policy in the United States. **E.P. Jackson***, C. Affeldt, J. Jackson, D.G. Kovacs

193. Stories of sustainability in communities: Bridging science and society. **E.P. Jackson***, D.G. Kovacs, J. Jackson

194. Development of green chemistry of synthetic fragrance/flavor substances. **F. Zheng***

195. The Green Chemistry Initiative at the University of Toronto. E.N. Daley, I. Malloj, J. Moir, L.M. Reyes, F. Tsao

196. Discovery of novel, potent, and low-toxic angiotensin II receptor type 1 (AT₁) blockers: Design, synthesis, biological evaluation, and molecular docking studies of 6-substituted aminocarbonyl benzimidazoles with a chiral center. **Z. Zhou***

Hawaii Convention Center
 303B

Active and Inquiry Learning in the Chemistry Classroom and Laboratory (#443)

Organized by: M. Buntine, S. Boniface, J. Lewis
Presiding: M. Buntine

19:00 – 197. Expert vs. novice: Can undergraduates ever become expert problem solvers? **T. Overton***

19:35 – 198. Supporting student understanding of chemistry through the use of guided inquiry materials and instructor facilitation. **R. Cole***, C. Stanford

19:50 – 199. Electrochemical sensors to detect heavy metals and carcinogenic compounds: Inquiry-based modules to meet today's interest. **S.K. Lunsford***, C. Spradlin, M. Sullivan

20:05 – 200. Enhancing student engagement in laboratory learning using inquiry-based activities: Expanding ASELL into schools. **A. Yeung***, M. Sharma, S. Kable, K.F. Lim, L. Sutherland, M. Buntine, V. Dawson, D. Southam, N. Maynard

20:20 – 201. Talking science: Productive student discourse in university-level chemistry courses. **D. Southam***, **G. Rushton**

20:35 – 202. Amalgamating flipped classroom and peer-led team learning pedagogies in general chemistry and organic chemistry instruction: An instructional experiment. **J.R. Raker**, S.E. Lewis, J. Antilla

20:50 Symposium close

Friday Morning

Hawaii Convention Center
 Halls I, II, III

Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113)

Organized by: R. Rogers, D. MacFarlane, R. Rogers, H. Ohno
Presiding: G. Gurau

Poster Session

10:00 – 12:00

203. Polyiodide formation in room temperature ionic liquids: 1-alkyl-3-methylimidazolium iodide. **H. Abe***, H. Kishimura, M. Aono, Y. Yoshimura, N. Hamaya

204. Hydrophobic ionic liquids for cellulose dissolution: Effect of respective alkyl chain length of cations and anions. **D. Sato**, K. Kuroda, M. Abe, H. Ohno

205. Electrocaryylation of aromatic ketones in ionic liquids: The Influence of the substrate and proton availability in ionic liquids on product distribution. **S.F. Zhao***, M. Horne, A.M. Bond, J. Zhang

206. Design and synthesis of amino-substituted task-specific ionic liquids for platinum group metal ions extraction. **A. Miyazaki***, K. Funaki, K. Kanie, A. Muramatsu

207. Design of ionic liquids to dissolve chitin without heating. **M. Shimo**, H. Ohno*, M. Abe

208. Ionic liquids based on cationic ruthenium sandwich complexes: Effects of substituents on the thermal properties. **T. Higashi**, A. Komurasaki, T. Ueda, T. Mochida*

209. Photoreactive organometallic ionic liquids containing the B(CN)₄ anion. **T. Ueda**, T. Mochida*

210. Acidity in protic ionic liquids studied by NMR spectroscopy. **M. Hasani***, C. Angell*

211. Control of surface wettability by ionic liquid interface. **T. Ono***

* Principle Author

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- 212.** Protic ionic liquids as direct dissolution solvents for lignocellulose based textile fiber production. **A.P. Parviainen***, A.W. King, I. Kilpeläinen, U. Liimatainen, H. Sixta, M. Hummel, R. Wahlström, A. Suurküki
- 213.** Ternary phase behavior of phytosterol ethoxylate, water, and imidazolium-based ionic liquids: Effect of alkyl chain length in cation and anion species on the phase behavior. **T. Misra***, K. Nakamura, R. Sekihara, T. Endo, K. Sakai, H. Sakai, M. Abe
- 214.** Development of environmental-benign ionic liquids with dissolution ability of cellulose. M. Yasui, **Y. Takagi***
- 215.** Development of environmental-benign teaching materials using ionic liquids. **R. Nishida**, Y. Takagi*
- 216.** Distribution of chemically modified cytochrome c in the ionic liquid/buffer biphasic system. **K. Ikeda**, K. Fujita, N. NAKAMURA*, H. Ohno
- 217.** Preparation and characterization of novel magnetic ionic liquids. **N. Fukui**, Y. Takagi*
- 218.** Improved performance of conducting-bridge random access memory using ionic liquids. **A. Harada**, H. Yamaoka, K. Watanabe, S. Kishida, K. Kinoshita, T. Nokami, T. Itoh
- 219.** Dynamic structure of *N,N*-diethyl-*N*-methyl-*N*-(2-methoxyethyl)ammonium tetrafluoroborate-water mixture. **K. Kaneko**, K. Sahara, Y. Yoshimura, A. Shimizu
- 220.** Sugar chain recognition of lectin stored in hydrated ionic liquid. **M. Sanada**, K. Fujita, H. Ohno*
- 221.** Design of self-organized soft materials changing their nanosegregated structures by the addition of acids or salts. **T. Matsumoto***, T. Ichikawa, T. Kato, H. Ohno
- 222.** Synthesis of an ionic liquid with hydrogenium cation encapsulated by crownether. **S. Takeoka**, A. Kitada, K. Fukami, K. Murase
- 223.** Which structures hinder the dissolution of lignocellulose in ionic liquids? **K. Yoshida**, H. Nonaka*
- 224.** Ionic liquids from cationic Ruthenium sandwich complexes with trialkoxybenzene ligands. **T. Ueda**, T. Mochida*
- 225.** Preparation and properties of cyclam complexes with the Ti_2N anion. **Y. Oba**, T. Mochida*
- 226.** Artificial neural networks and the melting temperature of imidazolium-type and ammonium-type ionic liquids. **J.O. Valderrama***
- 227.** Saccharification of biomass with zwitterion/acid composites (VI)- catalyst ability of sulfonic acid group. **S. Suzuki***
- 228.** Synthesis of polyureas from diamines and CO_2 activated by ionic liquids. **M. Yoneyama***
- 229.** Complete dissolution of woody biomass with tetra-*n*-butylphosphonium hydroxide aqueous solution and the effect of additives. **S. Yamamoto**, H. Ohno*
- 230.** Development of ionic liquids equipped with hetero-atom containing substituents for Li-ion batteries. **N. Handa**, K. Matsumoto, Y. Fukaya, T. Nokami*, T. Itoh*
- 231.** Design of zwitterions to show temperature-sensitive reversible phase change after adding water. **Y. Mieno**, H. Ohno*
- 232.** Ionic liquids formed from cationic metal-chelate complexes bearing ether side chains. **X. Lan**, H. Hosokawa, Y. Funasako, T. Mochida
- 233.** Role of ionic liquids in electroactive devices. **R. Sotoike**, T. Yasuda, M. Watanabe, M. Nakano, Y. Iwasa
- 234.** Development of temperature responsive polyelectrolyte hydrogels derived from polymerized ionic liquid. **A. Okafuji**, Y. Deguchi, Y. Kohno, H. Ohno*
- 235.** Effectiveness of ionic liquids for recovery process of useful substrates accumulated in cyanobacteria. **K. Fujita**, D. Kobayashi, N. NAKAMURA, H. Ohno
- 236.** Structural transition of proteins in condensed aqueous ionic liquid solutions. **T. Takekiyo***, E. Yamaguchi, Y. Yoshimura
- 237.** Suppression effect on insulin amyloid by the use of ionic liquids. **E. Yamaguchi***, T. Takekiyo, Y. Yoshimura
- 238.** Synthesis of cage-forming silicate polymers and evaluation as electrolyte (II) - solidification of protic ionic liquids. **K. Okuda**, M. Fujita, Y. Takeoka, M. Rikutaka
- 239.** Hydrated ionic liquids as effective solvent of renaturation of aggregated recombinant cellulase expressed in *Escherichia coli*. **M. Kajiyama**, K. Fujita, H. Ohno*
- 240.** Synthesis and characterization of ionic liquids as electrolytes for battery applications: Investigation of charge and discharge characteristics. **S. Horiochi***, M. Fujita, Y. Takeoka, M. Rikutaka
- 241.** Design of amino acid ionic liquids containing aspartic acid anion and their application as solvents for lyotropic liquid liquid crystals. **H. Takeuchi**, T. Ichikawa, M. Yoshiro, T. Kato, H. Ohno*
- Hawaii Convention Center
302A
- Technology and Assessment Strategies for Improving Student Learning in Chemistry (#132)**
- Organized by:* T. Holme, P. Mahaffy, M. Schultz
Presiding: M. Schultz
- 8:00** Adjust starting time
- 8:30 – 242.** Exploring the interrelationship between technology, instructional-styles, assessment strategies, and learner experiences. **B.M. McCollum***
- 8:50 – 243.** Screenscarts vs. simulations for chemistry learning. **D. Herrington***, R. Sweeder, J.R. VandenPlas
- 9:10 – 244.** Designing assessments to characterize both what students know and what they can do with that knowledge. **M.M. Cooper***
- 9:40** Break
- 10:00 – 245.** Using a web-based activity to enhance understanding of mole-mass calculations. **S.D. Woodgate***
- 10:20 – 246.** SoftChalk and iClickers combination in the chemistry classroom: 21st century pedagogy for 21st century learners. **G.P. Redd**, E.C. Gravely, T.O. Lewis
- 10:40 – 247.** Electronic lab notebooks in chemical education: The importance of the lab infrastructure to the optimal learning environment. **K. Alibiziati***
- 11:00 – 248.** Assessing the assessments: Evidencing and benchmarking student learning outcomes in Chemistry. **S. Schmid***, S. Bedford, A. Bridgeman, G. O'Brien, I. Jamie, K.F. Lim, S. Pyke, M. Schultz, D. Southam
- Hawaii Convention Center
302B
- Small Businesses Reaching Out for Market Share: Tool Kit and Success Stories (#185)**
- Organized by:* J. Sabol, D. Lainson, A. Blunn, W. Chung
Presiding: J. Sabol
- 8:00** Coffee and Conversation
- 8:30** Opening Remarks
- 8:35 – 249.** Enigma of job creation through entrepreneurial ventures: Need for a new structure. **P.J. Wyatt***
- 9:05 – 250.** Bootstrapping a chemical company in the steel city. **B. Bosley**, B. Bosley
- 9:35 – 251.** Innovative organic materials for highly efficient energy storage capacitors. **t. goodson***
- 10:05** Intermission
- 10:20 – 252.** Knowing what you've got, what you know, what you don't, how to protect it, and push the boundaries. **M. Clark***
- 10:50 – 253.** ABR: Finding strategic value in chemical process development. **A. Blunn***
- 11:20 – 254.** Starting up a technology company and sustaining through the valley of death. **A. Rahman***, J. Sabol
- 11:50 Closing Remarks**
- Hawaii Convention Center
303A
- Green and Sustainable Chemistry Education for Tomorrow's Citizens of the World (#334)**
- Organized by:* J. Jackson, F. Zheng, R. Resendes, D. Kovacs, J. Jackson, K. Saito
Presiding: D.G. Kovacs
- 8:00 – 255.** What is the value of an undergraduate certification in green chemistry? **D.G. Kovacs***
- 8:20 – 256.** Making greener chemistry choices at the University of Toronto. **A.P. Dicks***, L. Hoch, M. Mastronardi
- 8:45 – 257.** Green Chemistry Initiative: Promoting green chemistry across all levels of education. **L.M. Reyes**
- 9:05 – 258.** Berkeley Center for Green Chemistry: An interdisciplinary approach to education, research and engagement. **M.J. Mulvihill**
- 9:30** Break
- 9:40 – 259.** Pitching profitable projects and protecting the planet: Green chemistry outreach for an industry audience. **M.O. Clarke**
- 10:05 – 260.** Green chemistry education in Japan for tomorrow's citizens. **K. Ogino***
- 10:30 – 261.** Introducing middle school students to green nanoscience as a means toward protecting the environment. **S.O. Obare***
- 10:55 – 262.** Synthesis and mechanical testing of bioplastics and degradable polymers in the high school classroom as a mechanism to engage students in issues of sustainability. **J.E. Wissinger***, R. Harris, M. Yu, D. Schneiderman
- 11:15 – 263.** Chemistry, creativity, and sustainability. **M. Kirchoff***
- Hawaii Convention Center
Halls I, II, III
- Active and Inquiry Learning in the Chemistry Classroom and Laboratory (#443)**
- Organized by:* M. Buntine, S. Boniface, J. Lewis
Presiding: M. Buntine
- Poster Session**
10:00 – 12:00
- 264.** An international perspective on AP Chemistry course curriculum and pedagogy. **M. DeWane**
- 265.** Engaging our students in conversations on teaching and learning. **S. Brydges***
- 266.** Computer simulations and animations coupled with guided-inquiry tutorials to improve students' understanding of chemistry. **T.J. Greenbowe**, J.I. Gelder, M.R. Abraham
- 267.** Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach. **S. Riegel**
- 268.** Breaking down barriers to student learning in organic chemistry utilizing undergraduate teaching assistants and student-centered classroom activities. **R.M. Kissling***
- 269.** Teaching with a 3D printer: New hands-on models for active learning in organic and physical chemistry. **F.A. Carroll***, D.N. Blauch
- 270.** Effective S-STEM program at a small Mid-Atlantic liberal-arts college. **M.J. D'Souza***
- 271.** Incorporating authentic research in an optional component of the second semester organic laboratory course. **J.G. Gillmore**, T.L. Smith
- 272.** Debunking nuclear chemistry misconceptions using a POGIL activity and simulations. **M.L. Golden**, J. Wood, A. Lolino
- 273.** Bouncing batteries: Exploring the chemistry of alkaline cells. **J. Hall**, J. Amend, T. Kuntzleman
- Hawaii Convention Center
Halls I, II, III
- Connecting Chemistry to Society General Posters**
10:00 – 12:00
- Education and Teaching**
- 284.** Microscale experiments on various physicochemical properties of aqueous solutions for high school chemistry. **T. Nakagawa***
- 285.** Laser-induced breakdown spectroscopy for undergraduate chemistry research and teaching. **R.R. Hark**, A.I. Whitehouse
- 286.** Teaching online chemistry courses with a hands-on lab component. **R.R. Klepper***
- 287.** Infinity scholars, an NSF funded project that includes interdisciplinary undergraduate research. **R.R. Klepper***
- 288.** Content, concepts, context: first-year chemistry curriculum reform to improve both cognitive understanding and learning attitudes. **W. McNeil***, T.K. Freeman
- 289.** Role of faculty promotion in ensuring a successful first-year chemistry supplemental learning program. C.A. Bourne, S. McKeown, **T.K. Freeman***, W. McNeil
- 290.** Concerns with food and food labels. **M. Kurotani***, A. Yamamoto, M. Moriyama, M. shimizu, M. Shimamura
- Emerging Research Trends**
- 291.** Customized technology foresighting method. **D. Kim***, K. Choi
- 292.** Developing the integrated analysis of research trends called 4P analysis. **K. Choi***, D. Kim*

* Principle Author

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Friday Afternoon

Hawaii Convention Center
303A

Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113)

Organized by: R. Rogers, D. MacFarlane, R. Rogers, H. Ohno
Presiding: R.D. Rogers

13:00 Introduction

13:05 – 293. Can ionic liquids contribute to the world's energy economy?
J.S. Wilkes*

13:35 – 294. Using ionic liquids as a synthetic platform for energy conversion nanomaterials.
A.V. Mudring*

14:00 – 295. Durable and effective ionic liquids for a sustainable nuclear fuel cycle.
J.F. Wishart*, S. Dhiman, I.A. Shkrob

14:25 – 296. Specification and dynamics of alkali metal ions mixed salt/ionic liquid electrolytes: Toward improved Li and Na based energy storage.
M.S. Forsyth*, P. Howlett, H. Yoon, H. Zhu, L. O'Dell, D. MacFarlane

14:50 – 297. Development of functional ionic liquid-crystalline materials for energy and environment.
T. Kato*

15:15 – 298. Using ionic liquids to harvest waste heat.
J. Pringle*, D. Al-Masri, D. MacFarlane

15:40 – 299. Glyme-Li salt solvate ionic liquids for energy conversion and storage.
M. Watanabe*

16:05 – 300. Reversible photo-induced liquefaction and crystallization of ionic azobenzene derivatives with photon energy storage characteristics.
K. Ishiba, C. Chikara, M. Morikawa, T. Yamada, N. Kimizuka*

16:20 – 301. Ionic liquid lubrication technologies for energy generation systems.
S. Glavatskikh, O. Antzutkin

16:35 – 302. Phosphonium-based ionic liquids for energy storage devices.
C. Pozo-Gonzalo*, M. Forsyth, D. MacFarlane, P. Howlett

Hawaii Convention Center
302A

Technology and Assessment Strategies for Improving Student Learning in Chemistry (#132)

Organized by: T. Holme, P. Mahaffy, M. Schultz
Presiding: T. Holme

13:00 – 303. Use of written explanations to characterize student understanding of reaction mechanisms.
J.R. Raker

13:30 – 304. Investigation of video tutorial effectiveness and student use for general chemistry laboratories.
J.A. Key*, M. Paskevicius

13:50 – 305. Making the case: Why should others believe our assessment results?
J.E. Lewis*

14:20 Break
14:40 – 306. Formative assessment leading to self-directed learning in large, first-year chemistry classes.
M. Schultz*, G.A. Lawrie, S. Bedford, T. Dargaville, G. O'Brien, R. Tasker, M. Williams, A. Wright

15:10 – 307. Effective instruction medium for improving student learning of laboratory techniques.
J.P. Canal*, L. Hanlan, S. Lavieri, J. Lowe

15:30 – 308. Cyber-peer-led team learning (cPLTL).
P. Varma-Nelson*

15:50 – 309. What do we test vs. what do we want to test.
K. Murphy, T. Holme, C. Luxford

Hawaii Convention Center
302B

Small Businesses Reaching Out for Market Share: Tool Kit and Success Stories (#185)

Organized by: J. Sabol, D. Lainson, A. Blunn, W. Chung
Presiding: A. Blunn

13:00 Introductory Remarks

13:05 – 310. Creating innovation in an isolated region.
R. Melton

13:35 – 311. Inception sciences and the "build-to-buy" model: A novel paradigm for translation of emerging academic research into novel small molecule therapeutics.
B. Stearns*

14:05 – 312. Anybody can swim downstream: Get out of the fry pan, dance on the fire, and swim upstream.
J. Sabol

14:35 Intermission

14:50 – 313. ACS Committee on Corporation Associates and small chemical businesses.
N. Langerman*

15:20 – 314. Building businesses based on integration of basic and applied research: Value creation and new opportunities for chemists.
M.S. Chorghade*, R.S. Chorghade

15:50 – 315. Member benefits, programs, resources, and entrepreneurial activities from the ACS Division of Small Chemical Businesses SCHB.
J. Sabol

16:20 Concluding Remarks

Friday Evening

Hawaii Convention Center
303A

Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113)

Organized by: R. Rogers, D. MacFarlane, R. Rogers, H. Ohno
Presiding: G. Gurau

19:00 – 316. Improvement of electrochemical properties of electrolyte materials by addition of liquid zwitterions.
M. Fujita*, Y. Yamaguchi, Y. Takeoka, M. Rikukawa

19:15 – 317. Fundamental characterization of solvate ionic liquid/CO₂ binary system as electrolyte materials.
K. Watanabe*, T. Makino, M.L. Thomas, Y. Kamei, T. Mandai, M. Kanakubo, K. Dokko, M. Watanabe

19:30 – 318. Ionic liquid/polymer composites for low friction materials.
T. Sato*, T. Morinaga, T. Kamijo, H. Arafune, Y. Tsuji

19:45 – 319. Dicationsic imidazolium salts as a new class of organic ionic plastic crystals (OIPCs).
M. Lee*, H.W. Gibson

20:00 – 320. Task-specific ionic liquids: Using charge to your advantage for the selective extraction of rare earth elements.
N.J. Williams, C. Do-Thanh, J. Stankovich, H. Luo, S. Dai

20:15 – 321. Efficient decomposition of per-fluorinated ionic liquid anions to fluoride ions in subcritical and supercritical water.
H. Horii*, A. Takahashi

20:30 – 322. Organometallic ionic liquids from sandwich complexes: Liquid properties and chemical reactivities.
T. Mochida*, Y. Funasako, S. Hamada

20:45 – 323. Immobilized ionic liquid catalysts supported on solid supports for organic reactions.
T. Sasaki*, E.N. Kusumawati, K. Harada, L.A. Sari, B.M. Bhanage

Hawaii Convention Center
Halls I, II, III

Technology and Assessment Strategies for Improving Student Learning in Chemistry (#132)

Organized by: T. Holme, P. Mahaffy, M. Schultz

Presiding: M. Schultz

Organized by: T. Holme, P. Mahaffy, M. Schultz

Poster Session

19:00 – 21:00

324. Distinction of structural isomers of esters by hydroxamic acid iron (III) method.
S. Nogami*, M. Inoue

325. Rapid measurement of iodine value utilizing *N*-chlorosuccinimide.
S. Kobayashi*, M. Inoue

326. Development of experimental materials for stepwise oxidation of toluene.
M. Shimamura*, M. Inoue

327. Oxidation of vegetable oils utilizing photoradical initiator.
K. Osanai*, M. Inoue

328. Synthesis of esters utilizing acetyl salicylic acid as the reagent for acetylation.
H. Fujiwara*, M. Inoue

329. Chemistry education and research using the desktop NMR spectrometer: pico-Spin 80.
K. Hiroki*, H. Sawada, N. Yamashita

330. Small-scale experiments in chemical engineering for chemical education for undergraduates.
S. Ohki, Y. Konno, S. Kuwahara, K. Katayama*

331. Using web-based activities to study student facility with the acid-base conjugate pair concept.
S.D. Woodgate

Saturday Morning

Hawaii Convention Center
303A

Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113)

Organized by: R. Rogers, D. MacFarlane, R. Rogers, H. Ohno
Presiding: D. MacFarlane

8:00 – 332. Ionic liquid composite membranes for CO₂/light gas separations.
R.D. Noble, W. McDowell, M.G. Cowan, Z. Singh, D. Gin

8:25 – 333. Ionic liquid gas absorption - toward industrialization.
R. Fehrmann*, A. Riisager, A. Kunov-Kruse, P. Thomassen, H. Kolding, S. Mossin

8:50 – 334. Advanced CO₂ capture solvents and polymer materials from imidazoles and imidazolium cations.
J.E. Bara, D. Wallace, J.D. Roveda, M. Mittenthal, S. Yue

9:15 INTERMISSION

9:35 – 335. Sustainable materials for energy harvesting - how shrimp shell waste and ionic liquids can make an impact on today's society.
G. Gurau*, J.L. Shamshina, N. Abdul Faruk Khan, S.P. Kelley, P. Burton, R.D. Rogers

10:00 – 336. Adsorbents for uranium uptake from seawater: Toward sustainable nuclear energy.
C. Tsouris*, W. Liao, S. Das, R. Mayes, C. Janke, T. Saito, S. Dai, L. Kuo, G. Gill

10:20 – 337. Investigation of TODGA in ionic liquid for rare earth ion separation.
H. Luo*, S. Dai, J. Stankovich

10:35 – 338. Solvation dynamics and charge transfer in prototypical ionic liquid + conventional solvent mixtures: Experiment and simulation.
B. Conway, M. Liang, X. Zhang, M. Maroncelli*

10:55 – 339. Stability of penicillin G in ionic liquid and ionic liquid-based extraction.
Q. LIU, X. Liang, Y. Li, C. Zhang, H. Liu

11:10 – 340. Applications of switchable solvents in energy production and water purification.
P.G. Jessop*, M. Cunningham

Hawaii Convention Center
303A

Technology and Assessment Strategies for Improving Student Learning in Chemistry (#132)

Organized by: T. Holme, P. Mahaffy, M. Schultz
Presiding: S. Schmid

8:00 Adjust Starting Time

8:30 – 341. Exploring how students make sense of animations in variance in connection to experimental evidence.
R.M. Kelly*

8:50 – 342. Making learning smart through connections: Learnsmart and Connect in introductory general chemistry classes.
R. Venkateswaran*

9:10 – 343. Assessing high level skills in a chemistry context - the New Zealand Scholarship examination.
S. Boniface*

9:40 Break

10:00 – 344. Implementation of the computer version of the ACS General Chemistry Exam: A pilot study.
K.M. Elkins*, K. Murphy

10:20 – 345. Automated detection of problem-solving strategies from logs of student interactions with a virtual laboratory: A scalable approach to assessing inquiry skills.
D.J. Yaron*, Y. Gal, O. Uzan, R. Belford, M. Karabinos

10:40 – 346. Barriers and boundaries to e-learning in chemical and physical sciences.
I. Kooper

11:00 – 347. Automated alignment of instructor-created test items with the ACS Anchoring Concepts Content Map.
D.M. Hart*, T. Holme

Hawaii Convention Center
302B

Educational Approaches to Help Students Connect Chemistry to World Issues of Sustainability and Climate (#149)

Organized by: T. Holme, P. Mahaffy, M. Kirchhoff, M. Chiu, R. Kelly
Presiding: M. Kirchhoff

8:00 Starting time adjustment

8:30 – 348. CLEAR: Collaborative learning through environmental and aerosol research.
H. Weizman*, R. Pomeroy, K.N. Busby

8:50 – 349. Flipped classroom approach to increase student engagement with algal harmful metabolites separation from water.
L. Azouz*, A. Zamyadi, R. Stuetz, R.K. Henderson

9:10 – 350. Context or content? Both! (part 1).
C.H. Middlecamp*

9:40 Break

10:00 – 351. Context or content? Both! (part 2).
B.D. Fahlman

10:30 – 352. Using local environmental concerns to provide contexts to raise student interest in General Chemistry topics.
T. Holme

10:50 – 353. Hybridization of knowledge sets in middle-school students peer-group discourse during a scientific café on drinking water.
G.P. NICCOLAI*, C. Polo, K. Lund, C. Plantin

11:10 – 354. An international perspective on sustainability education.
G.M. Bodner

Hawaii Convention Center
303B

Advancing Sustainability: Catalyzing Interdisciplinary Scholarship for Green Chemistry (#383)

Organized by: R. Peoples, S. Maguire, M. Hearn

8:00 Opening Remarks

8:05 – 355. Green chemistry as institutional entrepreneurship.
S. Maguire*, C. Hardy

8:45 – 356. Push and pull: The role of regulation in advancing green chemistry.
T. Malloy*

* Principle Author

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9:25 – 357. Moving toward sustainable chemistry and engineering is an interdisciplinary necessity. **D.C. Constable**

9:45 Break

10:00 – 358. Greener solutions program: A private/public partnership advancing the design of safer chemistry. **M.J. Mulvihill, M. Schwarzman**

10:20 – 359. Green chemistry at McGill University: An experience of interdisciplinarity. **A. Moores, S. Maguire, C. Li, S. Ghoshal**

10:40 – 360. Knowledge commons for green chemistry. **A. Kokai*, A. Iles**

11:00 – 361. Fabrication of electrode materials for super-capacitor purposes prepared from graphite occurred by natural products. **M. Komatsu*, H. Okabayashi, K. Uehara**

11:20 – 362. Transparency in cleaning product formulation: What do we know about ingredients, their hazards, and potential for human exposure? **P. DeLeo*, E.S. Williams, M. Ciario, C. Pacelli, W. Greggs**

11:40 Q&A Plus Discussion

11:55 Closing Comments

Saturday Afternoon

Hawaii Convention Center
303A

Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113)

Organized by: R. Rogers, D. MacFarlane, R. Rogers, H. Ohno
Presiding: H. Ohno

13:00 – 363. Utilizing natural fiber welding for the fabrication of renewable biocomposite materials. **H. DeLong, E. Fox, D. Durkin, R. Russel, M. Brusoski, T. Price, E. Brown, P. Trulove**

13:25 – 364. Catalytic oxidation of lignin in ionic liquids: Is lignin a future alternative source for green chemicals?. **R.D. Singer*, B. Hurisso**

13:50 – 365. Development of phosphonate type ionic liquids having functional groups for biomass processing. **Y. Fukaya, R. Asai, T. Itoh***

14:05 – 366. Interfacial strategies for controlling nanoscale growth using ionic liquids. **G.A. Baker***

14:30 – 367. Functional ion gels. **T.P. Lodge***

14:55 Intermision

15:25 – 368. Transdermal delivery and pathogen neutralization with ionic liquids. **R. Del Sesto*, A. Koppisch, D.T. Fox, A. Newsham, M. Jones, T. Kern, M. Zakerwsky, S. Mitragotri**

15:50 – 369. Aqueous biphasic systems composed of ionic liquids: Remarkable purification platforms for biopharmaceuticals. **M.G. Freire***

16:15 – 370. Control of temperature-driven phase change of ionic liquid/water mixtures. **H. Ohno***

16:30 – 371. Reversible aqueous biphasic systems of polymers and ethanolamine-based ionic liquids. **M.G. Freire, J. Coutinho, A. Ferreira***

Hawaii Convention Center
302B

Technology and Assessment Strategies for Improving Student Learning in Chemistry (#132)

Organized by: T. Holme, P. Mahaffy, M. Schultz
Presiding: S. Boniface

13:00 – 372. Measuring meaningful learning in the undergraduate chemistry laboratory. **S. Bretz*, K.R. Galloway**

13:30 – 373. Development of chemistry instructional videos to improve first year students learning. **S. Lavieri*, J.P. Canal**

13:50 – 374. Identifying at-risk students in general and organic chemistry and in different institutional settings using cluster analysis of affective characteristics. **C. Bauer, J.Y. Chan*, A. Grushow**

14:20 Break

14:40 – 375. Using assessment to drive development of transferable skills. **T. Overton***

15:10 – 376. Assessing student preparation for general chemistry and student learning during the semester using ALEKS. **T. McGill*, D. Mulford**

15:30 – 377. Assessing assessment: How instructors use and understand information that chemistry tests provide. **T. Holme**

15:50 – 378. Evidencing learning in student-generated representations and explanations using web 2.0 technologies as vehicles for assessment. **G.A. Lawrie***

Hawaii Convention Center
302A

Historical Evolution of the Chemical Community in the Countries of the Pacific Rim (#198)

Organized by: S. Rasmussen, G. Patterson, I. Rae, Y. Furukawa, T. Levere
Presiding: S. Rasmussen

13:00 Introductory Remarks

13:05 – 379. Impact of the 1862 Morrill Land Grant College Act on chemistry education in the United States. **R.A. Egolf***

13:40 – 380. International relations of the Japanese chemical community. **Y. Kikuchi***

14:15 – 381. Out with the old, in with the new: Australian chemists and the United States of America. **I.D. Rae***

14:50 Break

15:00 – 382. Two centuries of chemistry in Canada. **T. Tidwell***

15:35 – 383. How the German PhD model crossed the Atlantic: Professionalization of American chemistry. **N. Heindel*, J. Sturchio**

16:10 – 384. Transformation of organic chemistry in Japan: From Majima Riko to the third international symposium on the chemistry of natural products. **M. Kaji***

Hawaii Convention Center
303B

Advancing Sustainability: Catalyzing Interdisciplinary Scholarship for Green Chemistry (#383)

Organized by: R. Peoples, S. Maguire, M. Hearn

13:00 Opening Comments

13:05 – 385. Green chemistry and advanced materials from renewable polymers: Education, research, and entrepreneurship to motivate the next generation of scientists. **R.D. Rogers***

13:45 Break

14:00 – 386. Technology-driven field convergence in the field of bioplastic. **I. Milne**

14:40 – 387. Role of psychology in combatting stress through green chemistry in the undergraduate chemistry laboratory. **V. Tucker*, I. Sidhwani, S. Chowdhary, N. Udgirkar**

15:00 – 388. Partnerships as a vehicle for system change in the chemical industry. **H. Lin*, I. stadtler, N. Antadze**

15:20 Q&A and Discussion

15:50 Closing Comments

Sunday Morning

Hawaii Convention Center
303A

Connecting Ionic Liquids to Societal Issues: Materials, Medicines, Energy, and Water (#113)

Organized by: R. Rogers, D. MacFarlane, R. Rogers, H. Ohno
Presiding: R.D. Singer

8:00 – 389. Transport properties of aprotic heterocyclic anion (AHA) ionic liquids for electrochemical applications. **J.F. Brennecke*, L. Sun**

8:25 – 390. 3D nanostructure of the EmIM TFSI – graphite interface as a function of potential and added electrolyte. **A. Elbourne, S. McDonald, K. Voitkovsky, G. Warr, R. Atkin***

8:50 – 391. Using MD simulation and different aggregation analysis tools to probe the distinctive interactions and structures of ionic liquids and their mixtures. **J. Canongia Lopes*, K. Shimizu, C. Bernardes**

9:15 – 392. Structure and transport in ionic liquids, mixtures, and at interfaces. **E.W. Castner***

9:40 – 393. Solute dynamics, how does it relate to ionic-liquid structure?. **J.C. Araque, S.K. Yadav, M. Shadeck, M. Maroncelli, C.J. Margulis***

10:05 INTERMISSION

10:35 – 394. *ILThermo* version 2.0: Archival storage and retrieval of thermophysical properties for ionic liquids. **J.W. Magee*, A. Kazakov, R. Chirico, V. Dilky, C. Muzny, K. Kroenlein, M. Frenkel**

11:00 – 395. Designing surfactants fit for purpose in ionic liquid systems. **G. Warr*, R. Atkin, H. Jlang, M. Araos, A. Dolan, T. Murphy, S. Imberti**

11:15 – 396. Application of impedance spectroscopy as a tool to identify critical temperature in thermoresponsive materials. **R. Vedaranjan*, K. Jain, S. Gupta, M. Watanabe, M. Ishikiriyama, N. Matsumi**

11:30 – 397. Solubility of H₂S and SO₂ in ionic liquids: Correlation and thermodynamic consistency of data. **J.O. Valderrama***

11:45 – 398. Ionic transport property in the binary systems consisting of glyme-lithium salt solvate ionic liquids and polymers. **Y. Kitazawa*, R. Kido, K. Iwata, K. Ueno, K. Dokko, M. Watanabe***

Hawaii Convention Center
302B

Educational Approaches to Help Students Connect Chemistry to World Issues of Sustainability and Climate (#149)

Organized by: T. Holme, P. Mahaffy, M. Kirchhoff, M. Chiu, R. Kelly
Presiding: T. Holme

8:00 Adjust start time

9:00 – 399. Environmental success stories: Major pollution problems that we have solved and how our past successes empower us for the future. **F.M. Dunnivant***

9:20 – 400. Guided inquiry learning materials on sustainability for two chemistry courses. **K.B. Aubrecht*, J.P. Hoffmann, A.K. Cassidy, H.J. Quigley**

9:40 – 401. Bringing real-world issues of sustainability to premedical organic chemistry. **J. Tripp***

10:00 Break

10:00 – 402. Energy and climate change presentation in undergraduate introductory chemistry textbooks. **R. Yoho, B. Vannali**

10:20 – 403. Taking the passenger seat: Student-driven discourse and argumentation in the chemistry classroom. **D. Ragland***

10:40 – 404. Sustainability, creativity, and chemical education in a research-based environment. **J.L. Blatti***

11:00 – 405. Can general chemistry education contribute meaningfully to global sustainability literacy? An exemplar using climate science as a rich context.

P. Mahaffy*, M. Towns, m. kirchoff, b. martin, I. Mckenzie, T. Holme

Hawaii Convention Center
302A

Historical Evolution of the Chemical Community in the Countries of the Pacific Rim (#198)

Organized by: S. Rasmussen, G. Patterson, I. Rae, Y. Furukawa, T. Levere
Presiding: S. Rasmussen

8:00 – 406. History of the modern chemistry doctoral program in mainland China. **V.V. Mainz**

8:35 – 407. Vehicles for discussion and publication of chemistry in 19th century Australia. **A.T. Baker***

9:10 – 408. History of the Korean Chemical Society. **G. Patterson**

9:45 – 409. Gen-itsu Kita and the Kyoto School's formation. **Y. Furukawa***

* Principle Author

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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INOR — Inorganic (2)
MACR — Macromolecular (3)
ORGN — Organic (4)

PHYS — Physical, Theoretical & Computational (5)
ENVR — Agrochemistry, Environmental and Geochemistry (6)

BIOL — Biological (7)
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PHYS — Physical, Theoretical &

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HLTH — Bench to Bedside: Chemistry

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KEY — PLEN — Plenary
ANYL — Analytical (1)
INOR — Inorganic (2)
MACR — Macromolecular (3)
ORGN — Organic (4)

PHYS — Physical, Theoretical &
Computational (5)
ENVR — Agrochemistry,
Environmental and Geochemistry (6)

BIOL — Biological (7)
MTLS — Materials & Nanoscience (8)
ENRG — Chemistry of Clean Energy Conversion,
Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary
ANYL — Analytical (1)
INOR — Inorganic (2)
MACR — Macromolecular (3)
ORGN — Organic (4)

PHYS — Physical, Theoretical & Computational (5)
ENVR — Agrochemistry, Environmental and Geochemistry (6)

BIOL — Biological (7)
MTLS — Materials & Nanoscience (8)
ENRG — Chemistry of Clean Energy Conversion, Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry of Health Care (10)
SCTY — Connecting Chemistry to Society (11)

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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

ANYL — Analytical (1)

Computational (5)

INOR — Inorganic (2)

ENVR — Agrochemistry,

MACR — Macromolecular (3)

Environmental and Geochemistry (6)

BIOL — Biological (7)

MTLS — Materials & Nanoscience (8)

ENRG — Chemistry of Clean Energy Conversion,

Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry

of Health Care (10)

SCTY — Connecting Chemistry to

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KEY — PLEN — Plenary
ANYL — Analytical (1)
INOR — Inorganic (2)
MACR — Macromolecular (3)
ORGN — Organic (4)

PHYS — Physical, Theoretical & Computational (5)
ENVR — Agrochemistry, Environmental and Geochemistry (6)

BIOL — Biological (7)
MTLS — Materials & Nanoscience (8)
ENRG — Chemistry of Clean Energy Conversion, Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry of Health Care (10)
SCTY — Connecting Chemistry to Society (11)

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 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
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BIOI — Biological (7)
 MTLS — Materials & Nanoscience (8)
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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

BIOL — Biological (7)

HLTH — Bench to Bedside: Chemistry

ANYL — Analytical (1)

Computational (5)

of Health Care (10)

INOR — Inorganic (2)

ENVR — Agrochemistry,

SCTY — Connecting Chemistry to

MACR — Macromolecular (3)

Environmental and Geochemistry (6)

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Society (11)

ORGN — Organic (4)

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
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 ENVR — Agrochemistry,
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BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical & Computational (5)
 ENVR — Agrochemistry, Environmental and Geochemistry (6)

BIOl — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion, Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry of Health Care (10)
 SCTY — Connecting Chemistry to Society (11)

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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

BIOL — Biological (7)

HLTH — Bench to Bedside: Chemistry

ANYL — Analytical (1)

Computational (5)

of Health Care (10)

INOR — Inorganic (2)

ENVR — Agrochemistry,

SCTY — Connecting Chemistry to

MACR — Macromolecular (3)

Environmental and Geochemistry (6)

Storage, and Production (9)

Society (11)

ORGN — Organic (4)

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KEY — PLEN – Plenary
 ANYL – Analytical (1)
 INOR – Inorganic (2)
 MACR – Macromolecular (3)
 ORGN – Organic (4)

PHYS – Physical, Theoretical &
 Computational (5)
 ENVR – Agrochemistry,
 Environmental and Geochemistry (6)

Biol – Biological (7)
 MTLS – Materials & Nanoscience (8)
 ENRG – Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH – Bench to Bedside: Chemistry
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 SCTY – Connecting Chemistry to
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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

BIOL — Biological (7)

HLTH — Bench to Bedside: Chemistry

ANYL — Analytical (1)

Computational (5)

of Health Care (10)

INOR — Inorganic (2)

ENVR — Agrochemistry,

SCTY — Connecting Chemistry to

MACR — Macromolecular (3)

Environmental and Geochemistry (6)

Storage, and Production (9)

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ORGN — Organic (4)

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PHYS — Physical, Theoretical &
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 ENVR — Agrochemistry,
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

Biol — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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MACR – Macromolecular (3)
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PHYS – Physical, Theoretical &
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ENVR – Agrochemistry,
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BIOL – Biological (7)
MTLS – Materials & Nanoscience (8)
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

Biol — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

ANYL — Analytical (1)

Computational (5)

INOR — Inorganic (2)

ENVR — Agrochemistry,

MACR — Macromolecular (3)

Environmental and Geochemistry (6)

BIOL — Biological (7)

MTLS — Materials & Nanoscience (8)

ENRG — Chemistry of Clean Energy Conversion,

Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry

of Health Care (10)

SCTY — Connecting Chemistry to

Society (11)

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

BIOL — Biological (7)

HLTH — Bench to Bedside: Chemistry

ANYL — Analytical (1)

Computational (5)

of Health Care (10)

INOR — Inorganic (2)

ENVR — Agrochemistry,

ENRG — Chemistry of Clean Energy Conversion,

SCTY — Connecting Chemistry to

MACR — Macromolecular (3)

Environmental and Geochemistry (6)

Storage, and Production (9)

Society (11)

ORGN — Organic (4)

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOl — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
 of Health Care (10)
 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
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 SCTY — Connecting Chemistry to
 Society (11)

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical & Computational (5)
 ENVR — Agrochemistry, Environmental and Geochemistry (6)

BIOl — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion, Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry of Health Care (10)
 SCTY — Connecting Chemistry to Society (11)

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KEY — PLEN — Plenary
ANYL — Analytical (1)
INOR — Inorganic (2)
MACR — Macromolecular (3)
ORGN — Organic (4)

PHYS — Physical, Theoretical &
Computational (5)
ENVR — Agrochemistry,
Environmental and Geochemistry (6)

BIOL — Biological (7)
MTLS — Materials & Nanoscience (8)
ENRG — Chemistry of Clean Energy Conversion,
Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
of Health Care (10)
SCTY — Connecting Chemistry to
Society (11)

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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical &
 Computational (5)
 ENVR — Agrochemistry,
 Environmental and Geochemistry (6)

BIOL — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion,
 Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry
 of Health Care (10)
 SCTY — Connecting Chemistry to
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KEY — PLEN — Plenary
 ANYL — Analytical (1)
 INOR — Inorganic (2)
 MACR — Macromolecular (3)
 ORGN — Organic (4)

PHYS — Physical, Theoretical & Computational (5)
 ENVR — Agrochemistry, Environmental and Geochemistry (6)

Biol — Biological (7)
 MTLS — Materials & Nanoscience (8)
 ENRG — Chemistry of Clean Energy Conversion, Storage, and Production (9)

HLTH — Bench to Bedside: Chemistry of Health Care (10)
 SCTY — Connecting Chemistry to Society (11)

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KEY — PLEN — Plenary

PHYS — Physical, Theoretical &

BIOL — Biological (7)

HLTH — Bench to Bedside: Chemistry

ANYL — Analytical (1)

Computational (5)

Materials & Nanoscience (8)

of Health Care (10)

INOR — Inorganic (2)

ENVR — Agrochemistry,

Chemistry of Clean Energy Conversion,

SCTY — Connecting Chemistry to

MACR — Macromolecular (3)

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KEY — PLEN — Plenary
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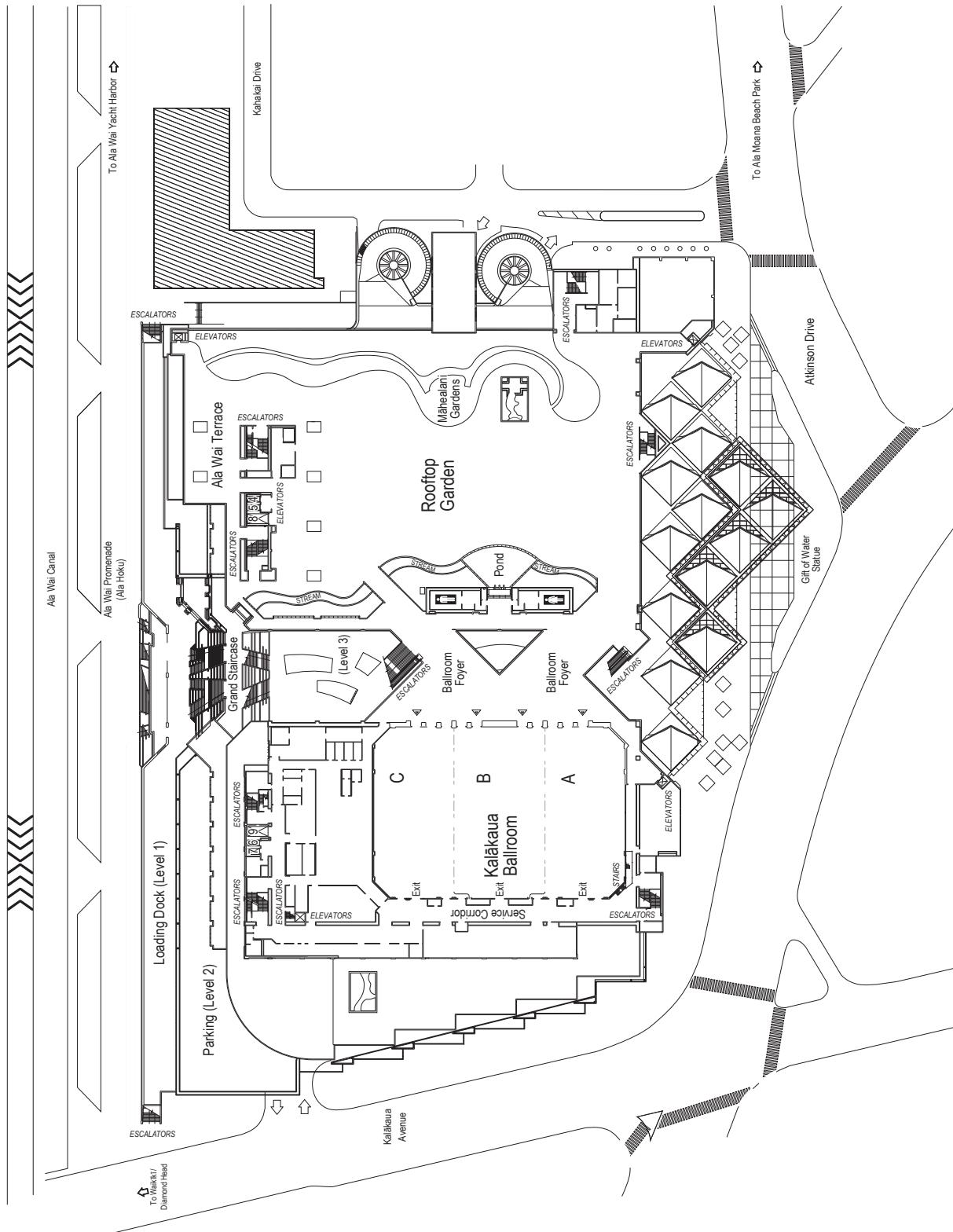
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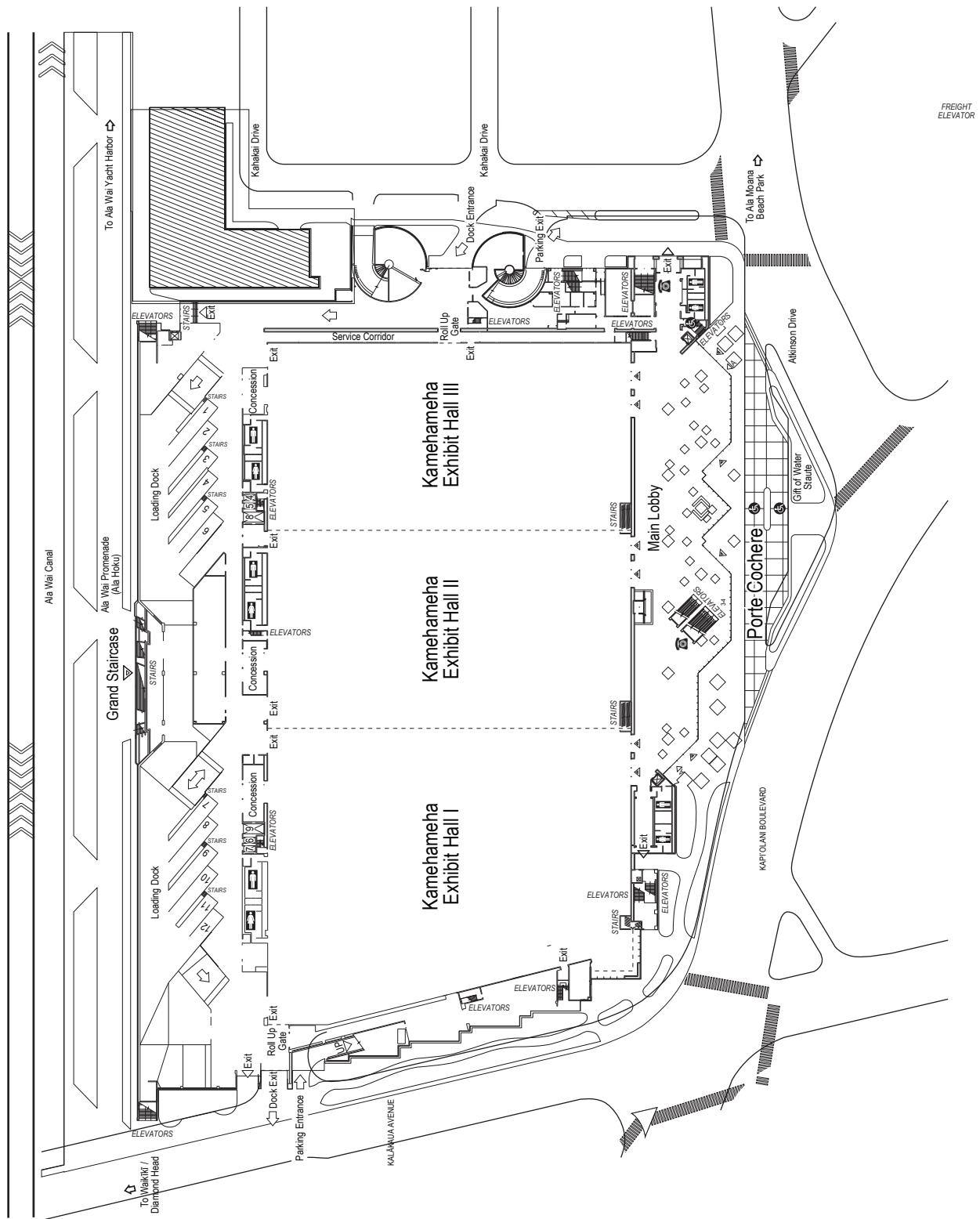
HAWAII CONVENTION CENTER

Ballroom & Parking Level



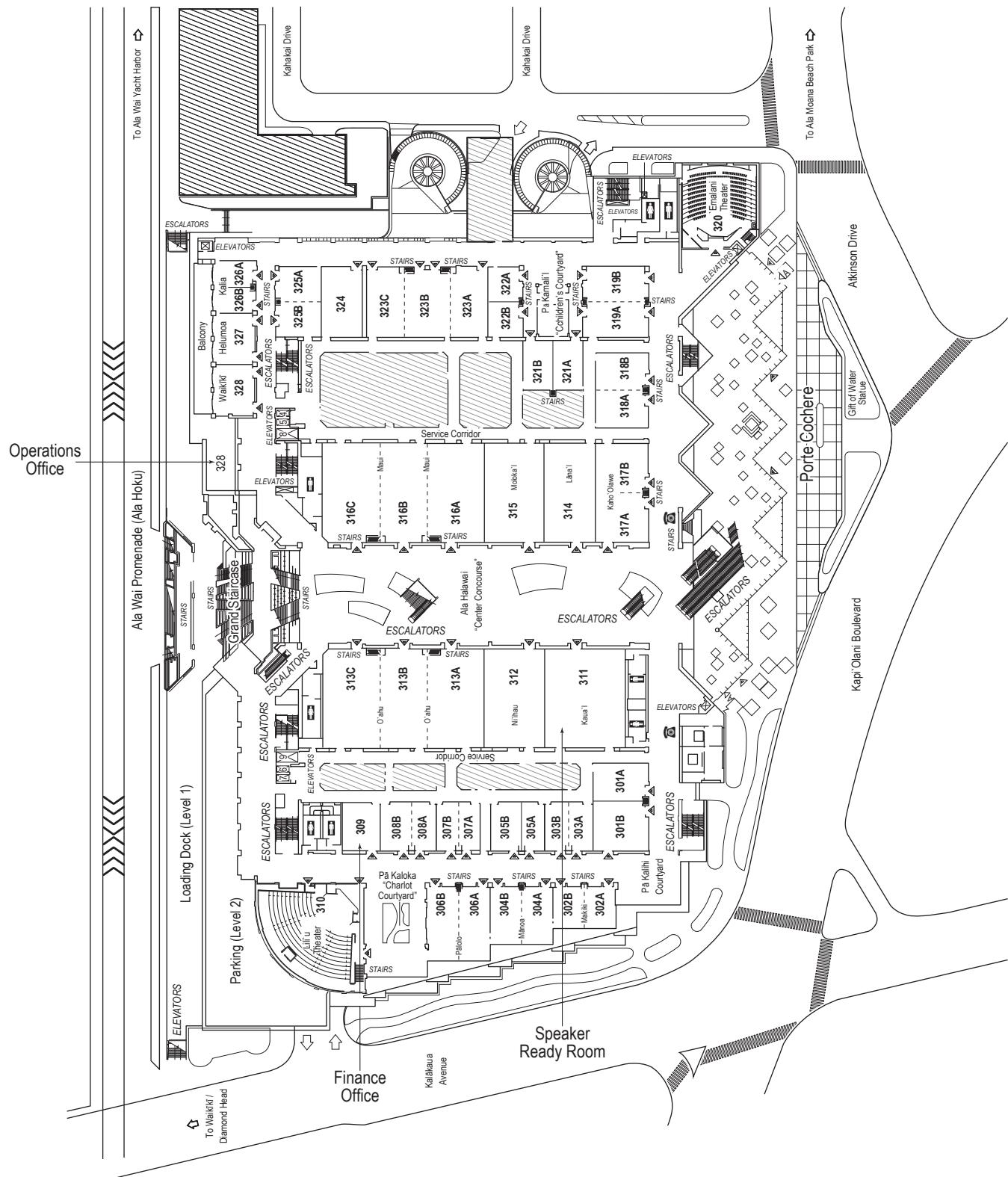
HAWAII CONVENTION CENTER

Exhibit Level



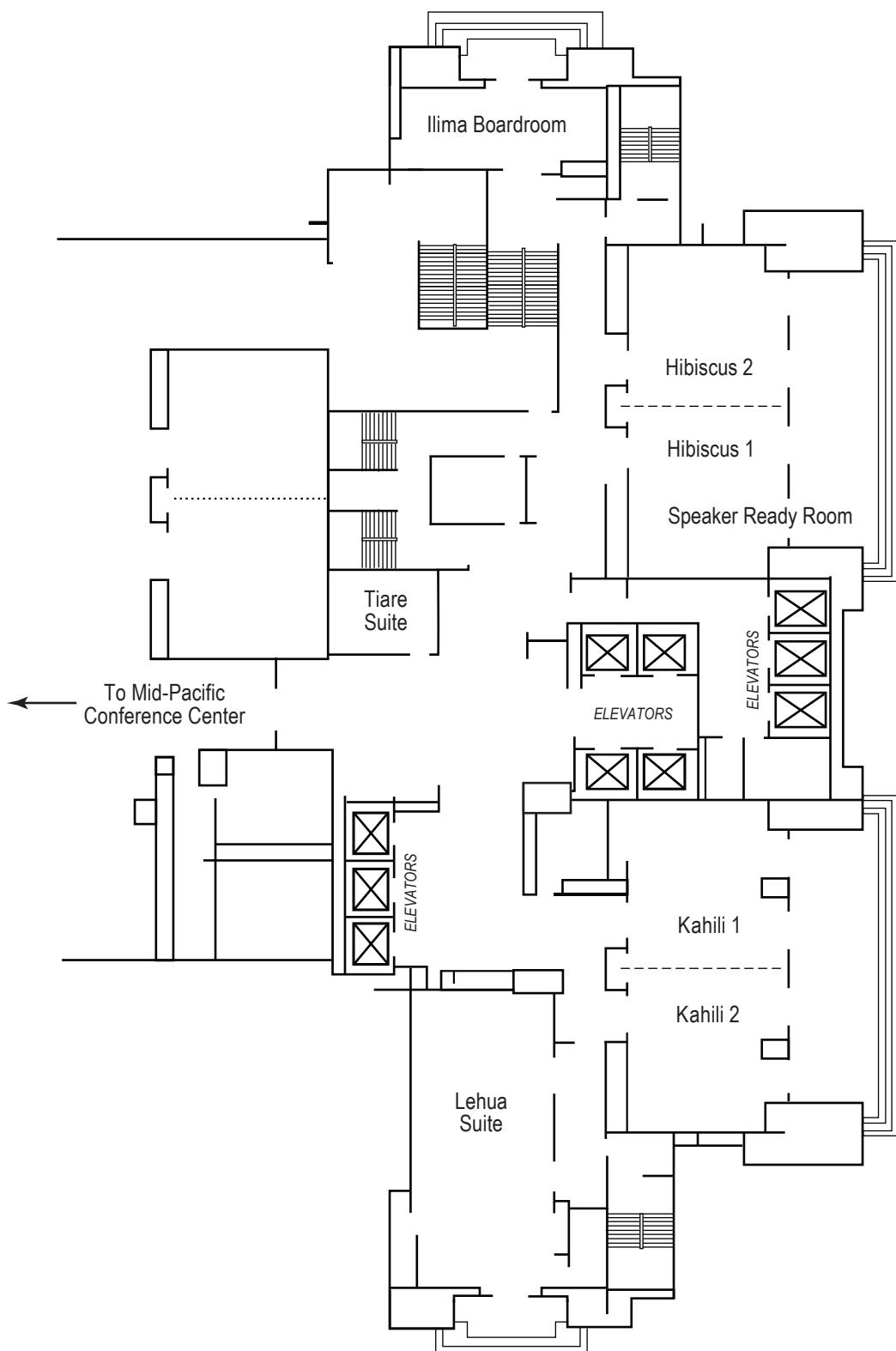
HAWAII CONVENTION CENTER

Meeting Room Level



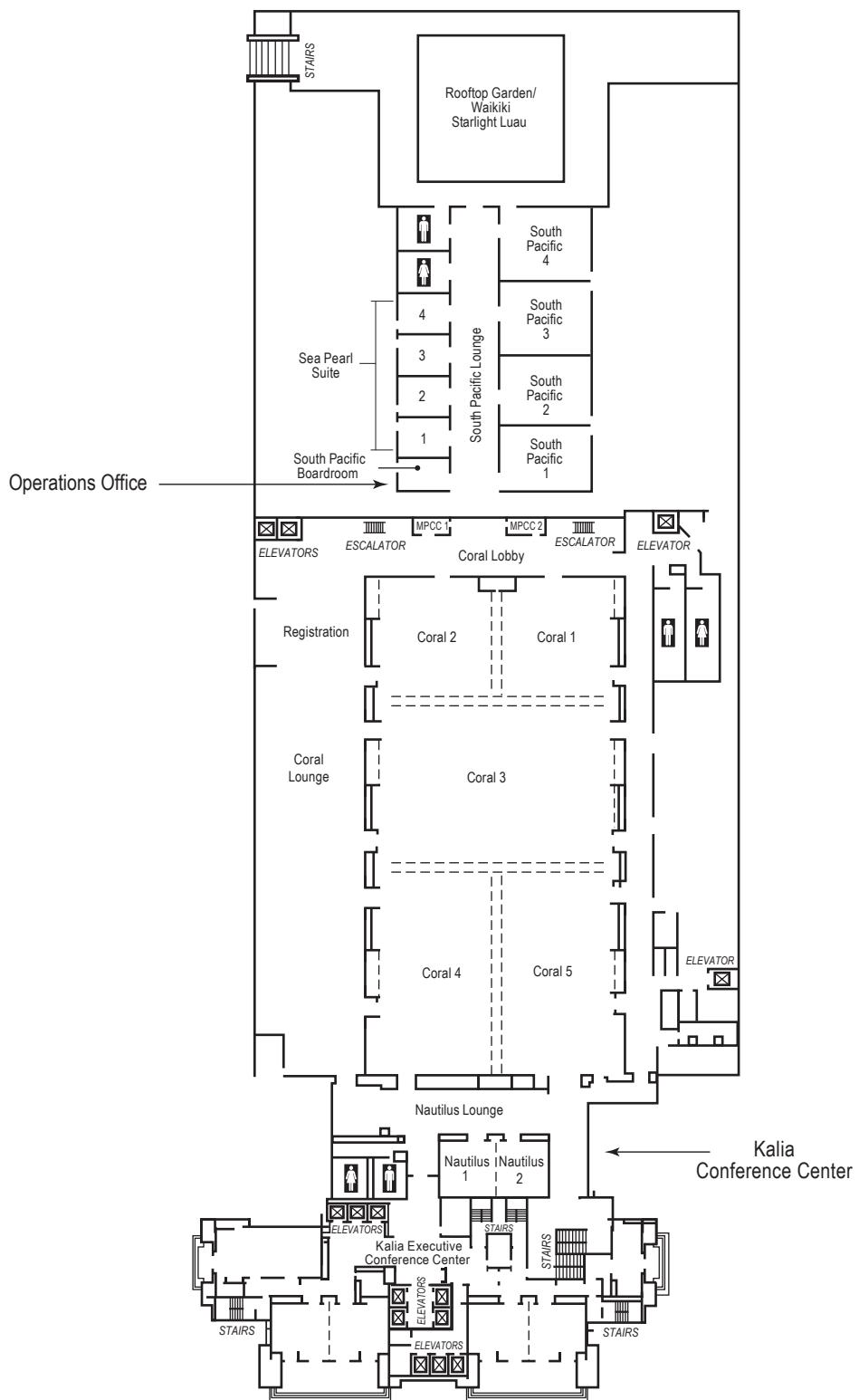
HILTON HAWAIIAN VILLAGE

Kalia Tower—Second Floor Kalia Conference Center



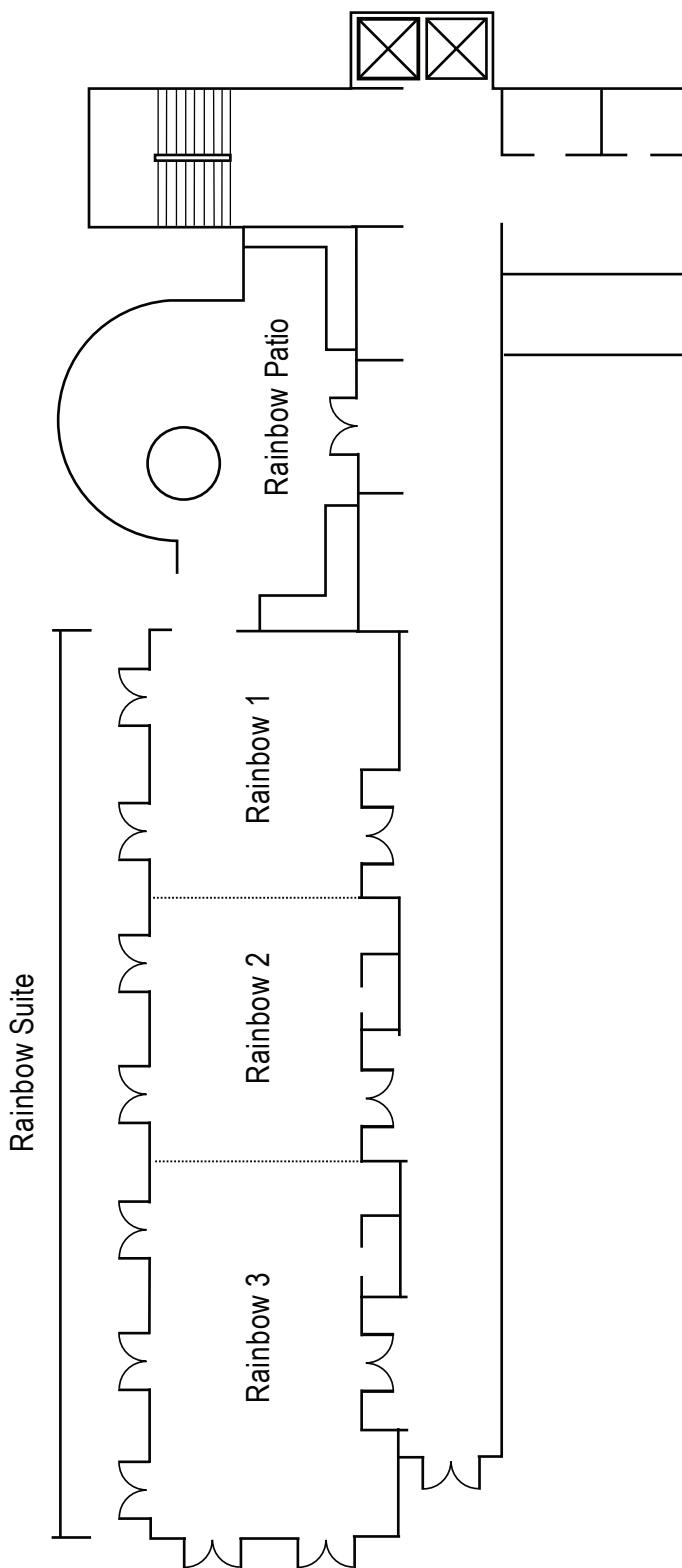
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Mid Pacific Conference—Sixth



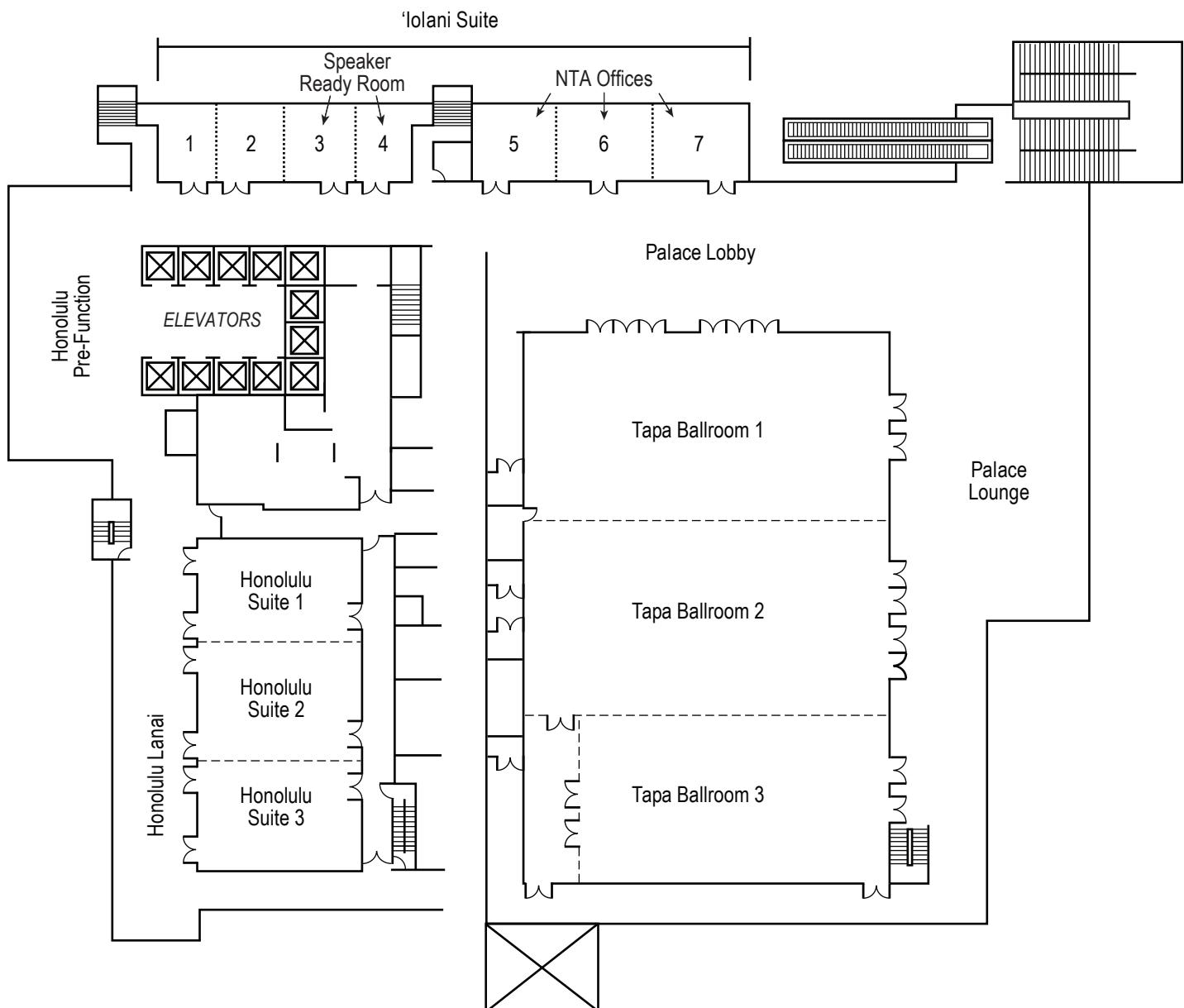
HILTON HAWAIIAN VILLAGE

Rainbow Tower-Lower Level



HILTON HAWAIIAN VILLAGE

Rainbow Tower—Second Floor

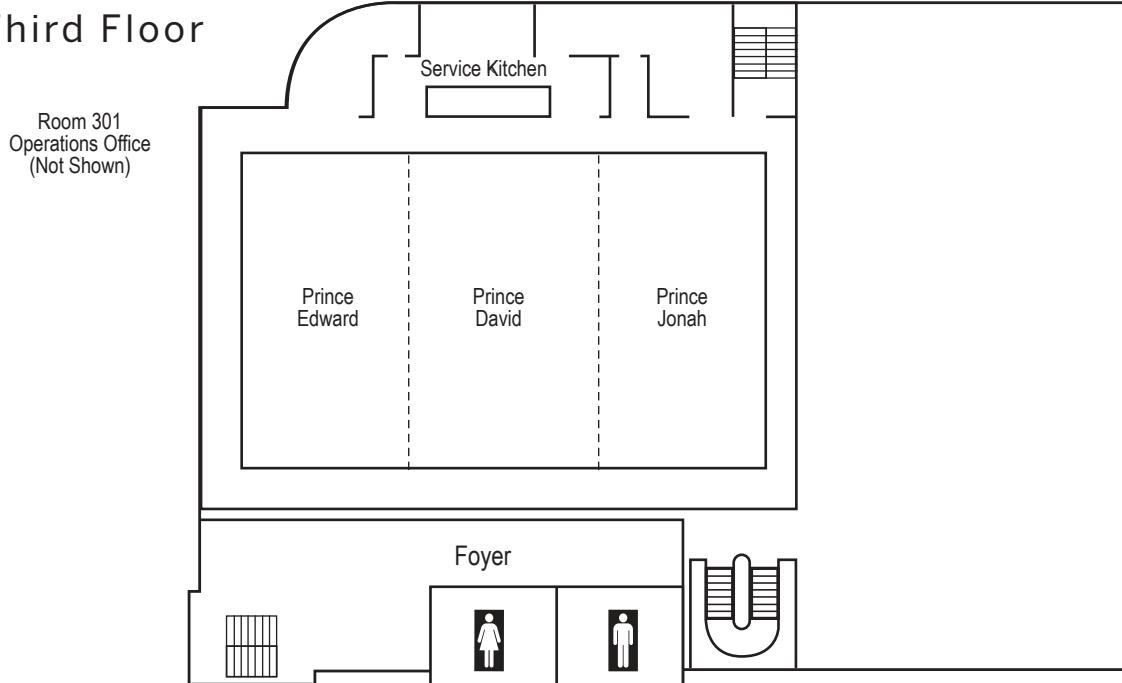


HILTON HAWAIIAN VILLAGE PROPERTY MAP

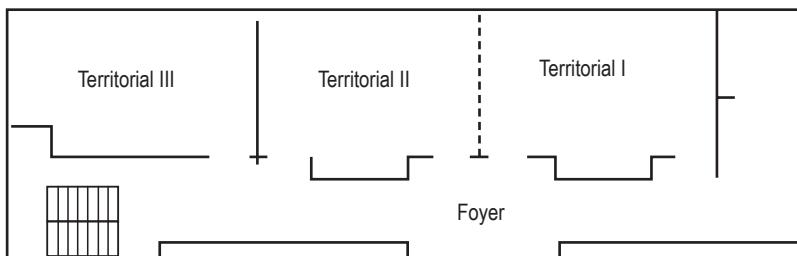


HILTON WAIKIKI BEACH

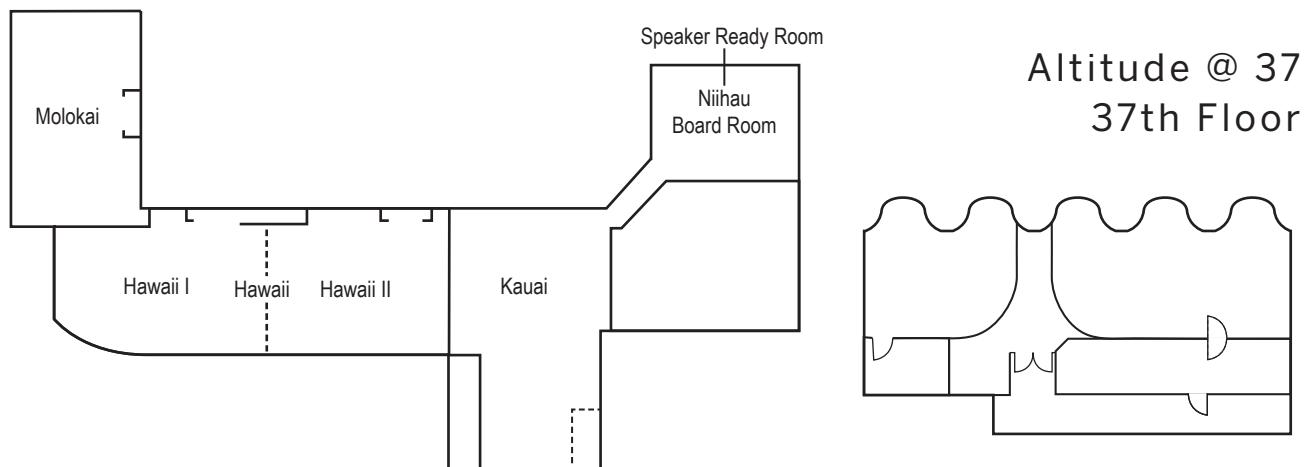
Third Floor



Fourth Floor

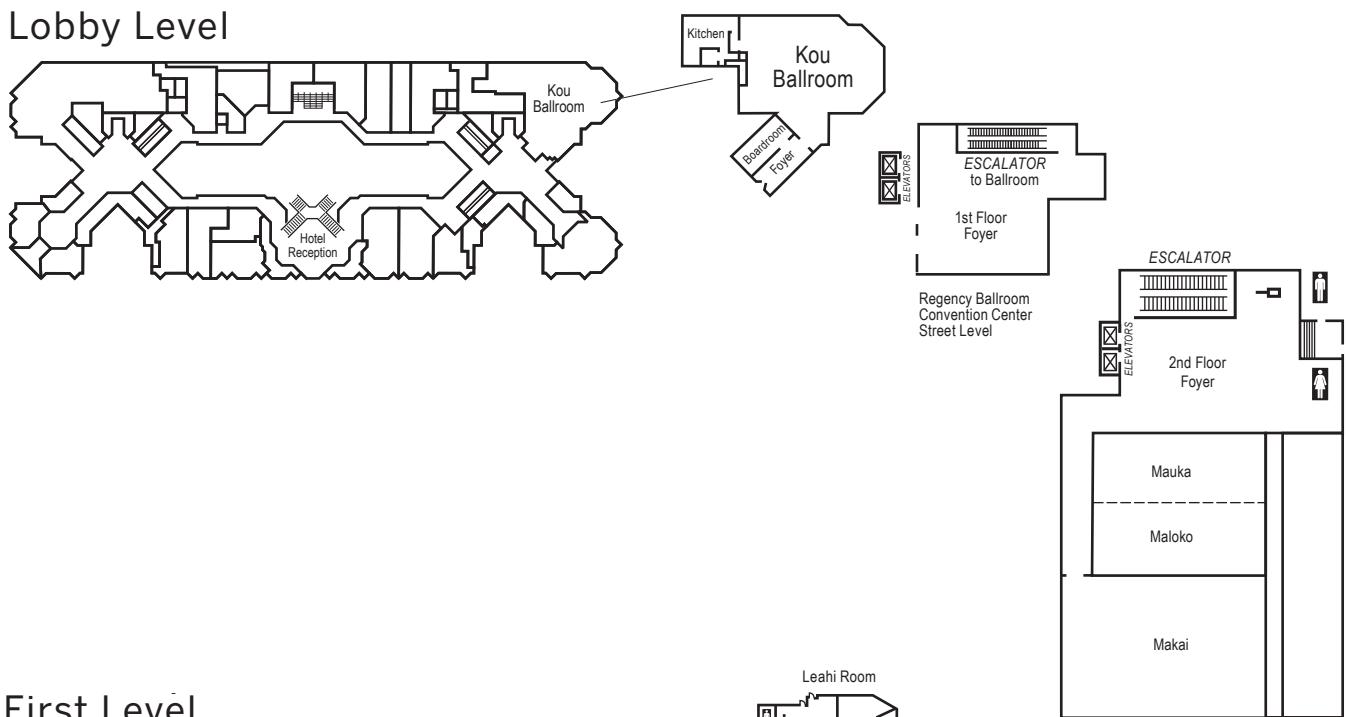


Second Floor

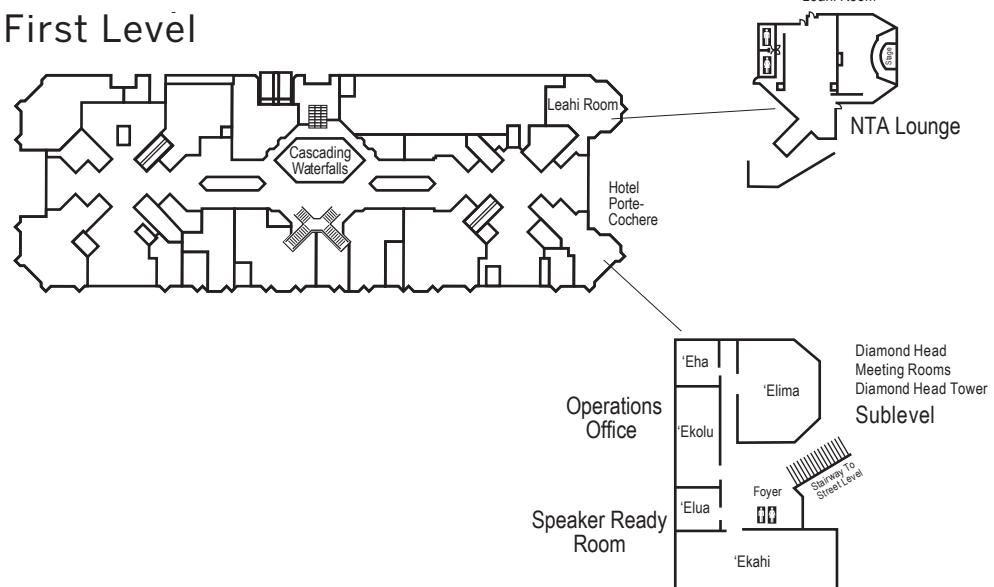


HYATT REGENCY WAIKIKI

Lobby Level

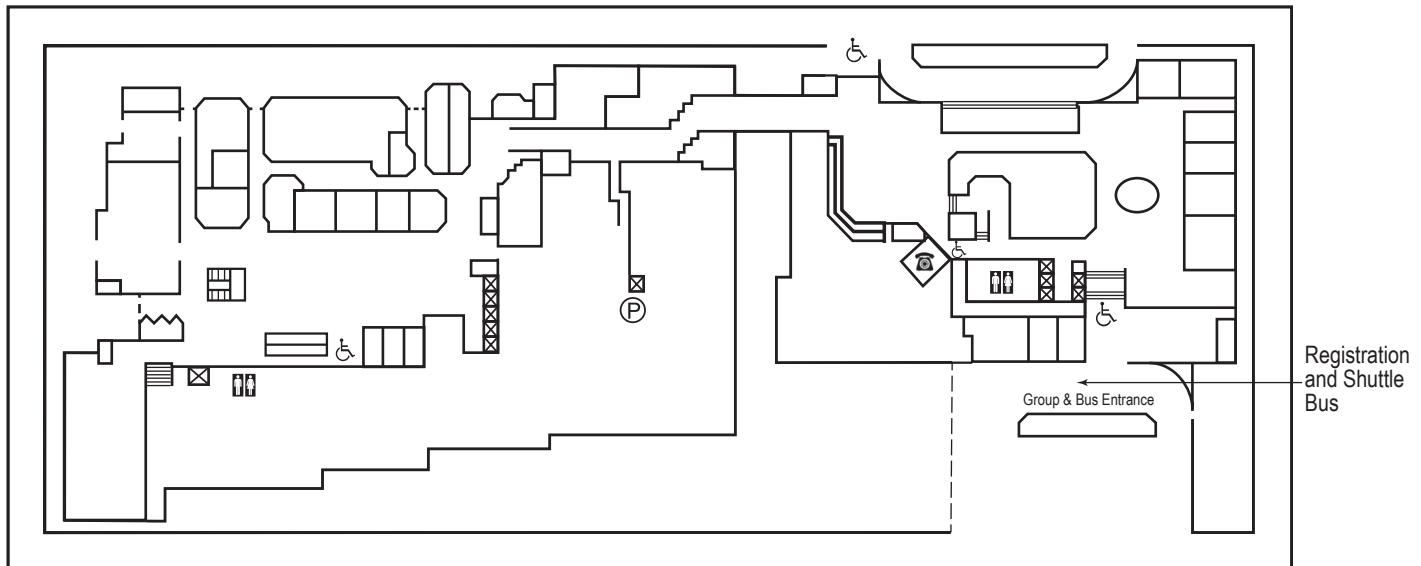


First Level

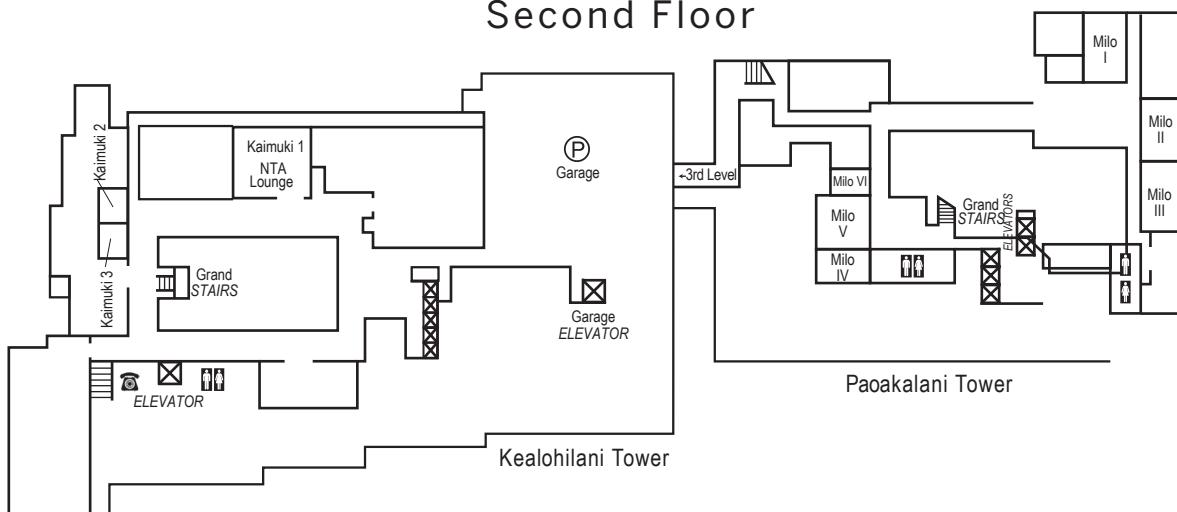


MARRIOTT RESORT WAIKIKI BEACH

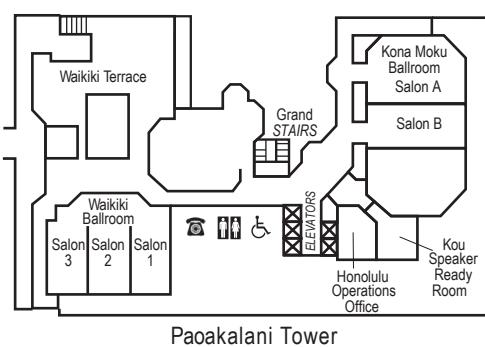
First Floor



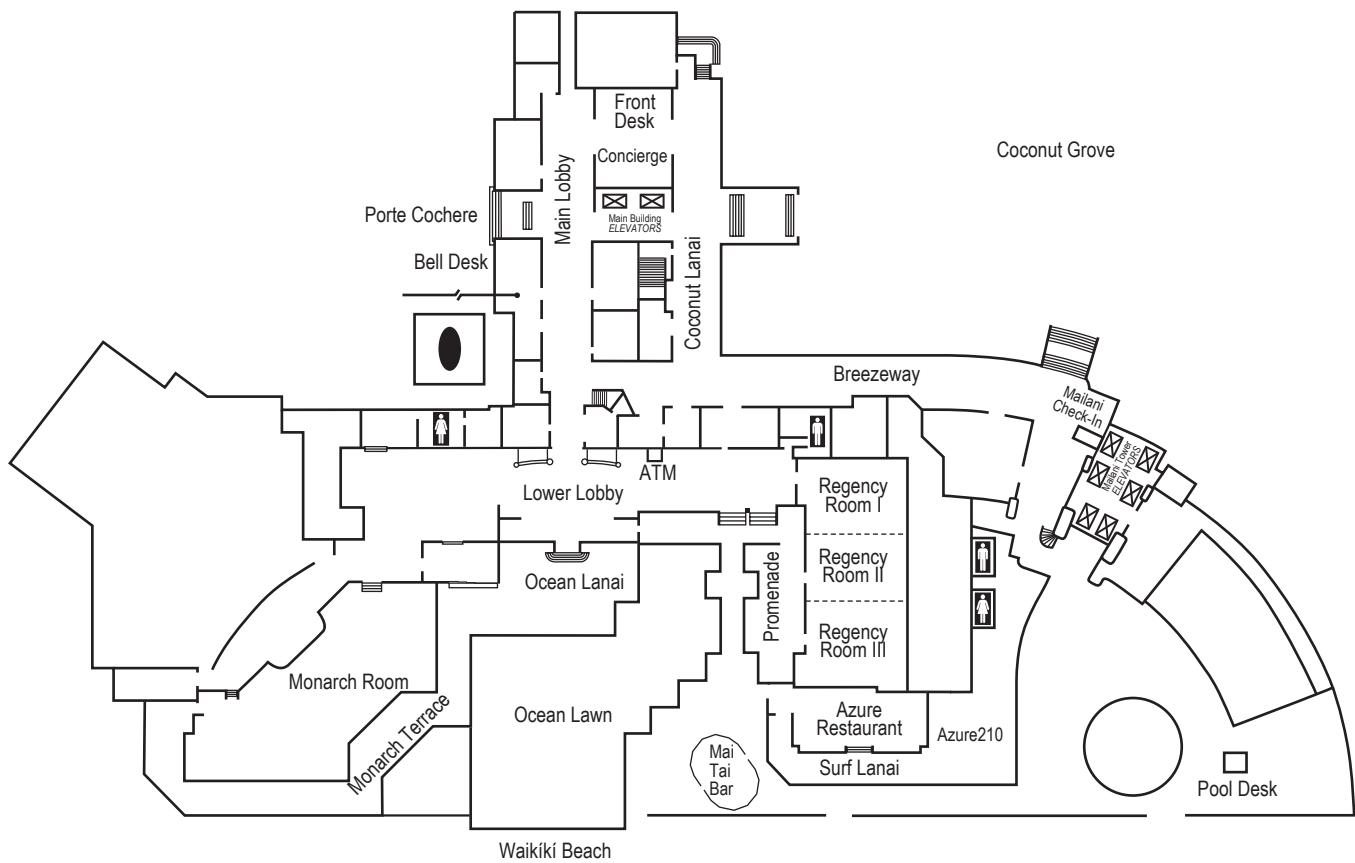
Second Floor



Third Floor

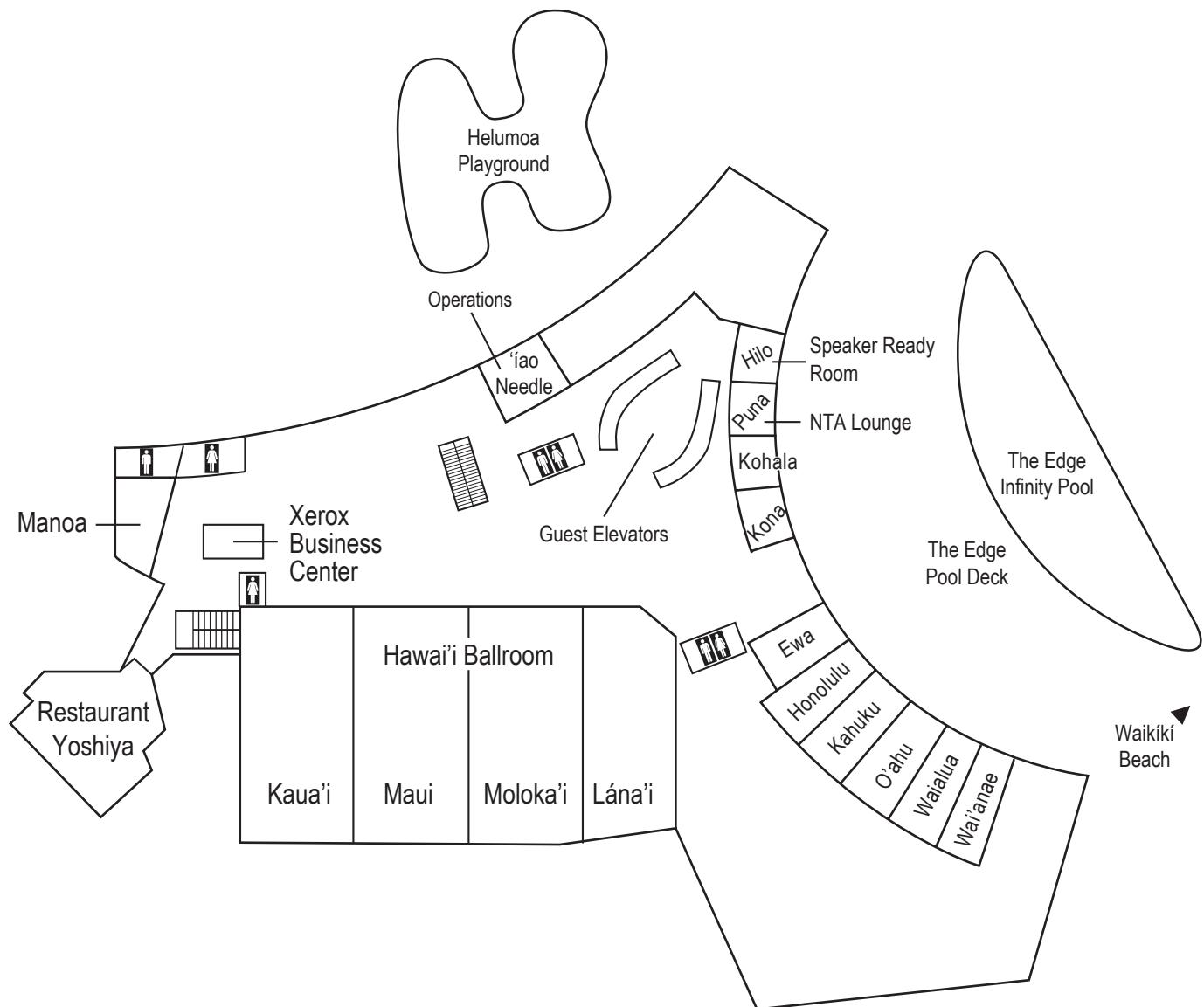


ROYAL HAWAIIAN



SHERATON WAIKIKI

Second Floor



PACIFICHEM OFFICIAL HOTELS

Ala Moana Hotel
410 Atkinson Drive
808-955-4811

Courtyard by Marriott Waikiki Beach
400 Royal Hawaiian Avenue
808-954-4000

DoubleTree by Hilton Alana Waikiki
1956 Ala Moana Blvd
808-941-7275

Embassy Suites Waikiki Beach Walk
201 Beachwalk Street
808-921-2345

Hawaii Prince Hotel Waikiki
100 Holomoana Street
808-956-1111

Hilton Hawaiian Village
2005 Kalia Road
808-949-4321

Hilton Waikiki Beach
2500 Kuhio Avenue
808-922-0811

Holiday Inn Resort Waikiki Beachcomber
2300 Kalakaua Avenue
808-922-4646

Hyatt Place Waikiki
175 Paoakalani Avenue
808-922-3861

Hyatt Regency Waikiki
2424 Kalakaua Avenue
808-923-1234

Marriott Waikiki Beach
2552 Kalakaua Avenue
808-922-6611

Outrigger Reef Waikiki Beach Resort
2169 Kalia Road
808-923-3111

Outrigger Waikiki Beach Resort
2335 Kalakaua Avenue
808-923-0711

Pacific Beach Hotel
2490 Kalakaua Avenue
808-922-1233

Ramada Plaza Waikiki
1830 Ala Moana Blvd
808-312-1148

Royal Hawaiian
2259 Kalakaua Avenue
808-923-7311

Sheraton Princess Kaiulani
120 Kaiulani Avenue
808-922-5811

Sheraton Waikiki
2255 Kalakaua Avenue
808-922-4422

The Modern Hotel
1775 Ala Moana Blvd.
808-450-3379

Trump International Waikiki Beach Walk
223 Saratoga Road
808-683-7777

Moana Surfrider
2365 Kalakaua Avenue
808-922-3111

PACIFICHEM OPERATION OFFICES

Hawaii Convention Center
Operations Office, Room 328,
808-792-6620

Hawaii Convention Center
Finance Office, Room 309,
808-792-6621

Hilton Hawaiian Village
Operations Office, South Pacific
Boardroom, 808-947-7939

Hilton Waikiki Beach
Operations Office, Room 301,
808-922-0811*

Hyatt Regency Waikiki
Operations Office, Ekolu Room,
808-947-7937

Marriott Waikiki Beach
Operations Office, Honolulu Room,
808-921-5036

Sheraton Waikiki
Operations Office, 'Iao Needle,
808-931-8091

*Ask for Pacifichem Operations
Office Room 301

Pacifichem 2015 Hotel Map



- 1 Ala Moana Hotel (C2)
- 2 Courtyard by Marriott Waikiki Beach (B7)
- 3 DoubleTree by Hilton Alana Waikiki (B4)
- 4 Embassy Suites Waikiki Beach Walk (D6)
- 5 Hawaii Prince Hotel Waikiki (D3)
- 6 Hilton Hawaiian Village Waikiki Beach (D4)
- 7 Hilton Waikiki Beach (B10)
- 8 Holiday Inn Resort Waikiki Beachcomber (C8)
- 9 Hyatt Place Waikiki (B11)
- 10 Hyatt Regency Waikiki Beach (C9)
- 11 Outrigger Reef (E6)
- 12 Outrigger Waikiki Beach Resort (D8)
- 13 Pacific Beach Hotel (C10)
- 14 Ramada Plaza Waikiki (C3)
- 15 Royal Hawaiian (E8)
- 16 Sheraton Princess Kaiulani (C9)
- 17 Sheraton Waikiki (E7)
- 18 The Modern Hotel (D3)
- 19 Trump International Waikiki Beach Walk (D6)
- 20 Waikiki Beach Marriott (C10)
- 21 Westin Moana Surfrider (D8)
- ★ Shuttle Pickup Locations



PARTICIPATING HOTEL LIST

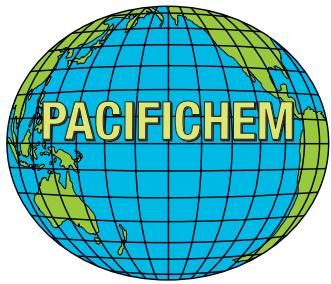
For best availability, make your reservation via the Internet at www.pacifichem.org or by phone at (866) 847-8570.

* All Pacificchem 2015 room rates include complimentary in-room Internet and fitness center access. Room rates below do not include 13.9% room tax (subject to change). **Additional fees may apply: if a rollaway bed is required, if there are pets in guest rooms, and if smoking occurs in guest rooms (all rooms are nonsmoking rooms). All hotels will have access to a shuttle route.

| HOTELS | Single | Double | Triple | Quad | **Max Guests/Room | Child Under Age Free | Childcare List | Parking | Room Service | ** Pets | Pool | ADA | Green Hotel |
|--|--------|--------|--------|-------|-------------------|----------------------|----------------|-----------|--------------|---------|------|-----|-------------|
| 1.a Ala Moana Hotel – Waikiki Tower | \$169 | \$169 | \$219 | \$269 | 4 | 17 | No | \$20/\$25 | No | No | Yes | Yes | Yes |
| 1.b Ala Moana Hotel – Kona Tower | \$149 | \$149 | N/A | N/A | 2 | 17 | No | \$20/\$25 | No | No | Yes | Yes | Yes |
| 2.a Courtyard by Marriott Waikiki – Standard Room | \$179 | \$179 | N/A | N/A | 2 | 17 | No | \$35 | No | No | Yes | Yes | No |
| 2.b Courtyard by Marriott Waikiki – Deluxe Room | \$189 | \$189 | \$214 | \$239 | 4 | 17 | No | \$35 | No | No | Yes | Yes | No |
| 2.c Courtyard by Marriott Waikiki – One Bedroom Suite | \$199 | \$199 | \$224 | \$249 | 4 | 17 | No | \$35 | No | No | Yes | Yes | No |
| 3 DoubleTree by Hilton Alana Waikiki | \$195 | \$195 | \$235 | \$275 | 4 | 17 | No | \$30 | Yes | Service | Yes | Yes | Yes |
| 4 Embassy Suites Waikiki | \$289 | \$289 | \$349 | \$409 | 4 | 18 | No | \$35 | Yes | Service | Yes | Yes | Yes |
| 5 Hawaii Prince Hotel Waikiki | \$195 | \$195 | \$255 | N/A | 3 | 18 | Yes | \$22/\$28 | Yes | Service | Yes | Yes | Yes |
| 6.a Hilton Hawaiian Village – Resort View | \$220 | \$220 | \$270 | \$320 | 4 | 17 | Yes | \$27/\$33 | No | Service | Yes | Yes | Yes |
| 6.b Hilton Hawaiian Village – Ocean View | \$255 | \$255 | \$305 | \$355 | 4 | 17 | Yes | \$27/\$33 | No | Service | Yes | Yes | Yes |
| 6.c Hilton Hawaiian Village – Deluxe Ocean Rainbow | \$285 | \$285 | \$335 | \$385 | 4 | 17 | Yes | \$27/\$33 | No | Service | Yes | Yes | Yes |
| 6.d Hilton Hawaiian Village – Ocean View Ali'i | \$310 | \$310 | \$360 | \$410 | 4 | 17 | Yes | \$27/\$33 | No | Service | Yes | Yes | Yes |
| 7.a Hilton Waikiki Beach – City or Mountain View | \$189 | \$189 | \$229 | \$269 | 4 | 17 | Yes | \$25 | Yes | Service | Yes | Yes | Yes |
| 7.b Hilton Waikiki Beach – Ocean View | \$239 | \$239 | \$279 | \$319 | 4 | 17 | Yes | \$25 | Yes | Service | Yes | Yes | Yes |
| 8 Holiday Inn Waikiki Beachcomber | \$189 | \$189 | \$239 | \$289 | 4 | 19 | No | \$35 | No | Service | Yes | Yes | Yes |
| 9 Hyatt Place Waikiki | \$239 | \$239 | \$254 | \$269 | 4 | 17 | No | \$25/\$30 | Yes | Yes | Yes | Yes | Yes |
| 10.a Hyatt Regency Waikiki Beach – City/Mountain View | \$230 | \$230 | \$305 | \$380 | 4 | 18 | Yes | \$30/\$35 | Yes | Yes | Yes | Yes | Yes |
| 10.b Hyatt Regency Waikiki Beach – Ocean View | \$250 | \$250 | \$325 | \$400 | 4 | 18 | Yes | \$30/\$35 | Yes | Yes | Yes | Yes | Yes |
| 11.a Outrigger Reef Waikiki Beach – Standard View | \$229 | \$229 | \$304 | N/A | 3 | 17 | Yes | \$35 | Yes | Service | Yes | Yes | Yes |
| 11.b Outrigger Reef Waikiki Beach – Partial Ocean View | \$259 | \$259 | \$334 | N/A | 3 | 17 | Yes | \$35 | Yes | Service | Yes | Yes | Yes |
| 12 Outrigger Waikiki Beach | \$235 | \$235 | \$305 | \$380 | 4 | 17 | Yes | \$35 | Yes | Service | Yes | Yes | Yes |
| 13 Pacific Beach Hotel | \$199 | \$199 | \$249 | \$299 | 4 | 17 | No | \$25/\$33 | Yes | Service | Yes | Yes | Yes |
| 14 Ramada Plaza Waikiki | \$149 | \$149 | \$179 | \$209 | 4 | 21 | No | \$25 | No | No | Yes | Yes | Yes |
| 15 Royal Hawaiian | \$275 | \$275 | \$375 | \$475 | 4 | 17 | Yes | \$25/\$33 | Yes | No | Yes | Yes | No |
| 16.a Sheraton Princess Kaiulani – City View | \$165 | \$165 | \$215 | \$265 | 4 | 17 | Yes | \$25 | Yes | No | Yes | Yes | No |
| 16.b Sheraton Princess Kaiulani – Ocean View | \$180 | \$180 | \$230 | \$280 | 4 | 17 | Yes | \$25 | Yes | No | Yes | Yes | No |
| 17.a Sheraton Waikiki – City View | \$229 | \$229 | \$304 | \$379 | 4 | 17 | Yes | \$25/\$33 | Yes | No | Yes | Yes | No |
| 17.b Sheraton Waikiki – Mountain View | \$245 | \$245 | \$320 | \$395 | 4 | 17 | Yes | \$25/\$33 | Yes | No | Yes | Yes | No |
| 17.c Sheraton Waikiki – Partial Ocean View | \$259 | \$259 | \$334 | \$409 | 4 | 17 | Yes | \$25/\$33 | Yes | No | Yes | Yes | No |
| 17.d Sheraton Waikiki – Ocean View | \$279 | \$279 | \$354 | \$429 | 4 | 17 | Yes | \$25/\$33 | Yes | No | Yes | Yes | No |
| 18.a The Modern Honolulu – City View | \$269 | \$269 | \$334 | \$399 | 4 | 18 | Yes | \$28 | Yes | Yes | Yes | Yes | No |
| 18.b The Modern Honolulu – Partial Ocean View | \$289 | \$289 | \$354 | \$419 | 4 | 18 | Yes | \$28 | Yes | Yes | Yes | Yes | No |
| 19 Trump International Hotel Waikiki | \$369 | \$369 | \$469 | \$569 | 4 | 19 | Yes | \$33 | Yes | Service | Yes | Yes | Yes |
| 20.a Waikiki Beach Marriot – City View | \$219 | \$219 | \$259 | \$319 | 4 | 17 | No | \$32/\$37 | Yes | Service | Yes | Yes | Yes |
| 20.b Waikiki Beach Marriot – Partial Ocean View | \$239 | \$239 | \$279 | \$319 | 4 | 17 | No | \$32/\$37 | Yes | Service | Yes | Yes | Yes |
| 21 Westin Moana Surfrider | \$245 | \$245 | N/A | N/A | 2 | 17 | Yes | \$25/\$40 | Yes | Service | Yes | Yes | No |

Orchid Event Solutions is the ONLY designated housing provider for Pacificchem 2015. Beware of companies misrepresenting themselves as affiliated with Pacificchem.





2015 International Chemical Congress of Pacific Basin Societies



Shuttle Boarding Locations & Schedules

ADA Assistance: Contact Naomi Aquino for reservations at least 7 days in advance at naomi.aquino@robertshawaii.com, cc: groupsales@robertshawaii.com or call 888-472-4729 or 808-539-9481. Call the dispatch hot line for same day request at 808-831-1555 (may incur a 30 minute wait time).

| ROUTE | HOTELS | BOARDING LOCATIONS |
|-------|----------------------------|--|
| 1 | Hawaii Prince | Tapa Front Bus Stop |
| | Hilton Hawaiian Village | Tapa Front Bus Stop |
| | Doubletree Alana | Front of Convention Center |
| | The Modern | Tapa Front Bus Stop |
| | Ramada Plaza | Front of Convention Center |
| | Convention Center | Front of Convention Center |
| 2 | Holiday Inn Beachcomber | Sheraton Bus Depot |
| | Sheraton Waikiki | Sheraton Bus Depot |
| | Embassy Suites | Sheraton Bus Depot |
| | Royal Hawaiian | Sheraton Bus Depot |
| | Trump Waikiki Beach Walk | Sheraton Bus Depot |
| | Westin Moana Surfrider | Sheraton Bus Depot |
| | Outrigger | Sheraton Bus Depot |
| | Outrigger Reef | Sheraton Bus Depot |
| | Courtyard Marriott | Sheraton Bus Depot |
| | Convention Center | Front of Convention Center |
| 3 | Hyatt Regency Waikiki | Hyatt Koa Ave Entrance |
| | Pacific Beach Hotel | Hyatt Koa Ave Entrance |
| | Sheraton Princess Kaiulani | Hyatt Koa Ave Entrance |
| | Convention Center | Front of Convention Center |
| 4 | Hyatt Place | Marriott Bus Depot |
| | Waikiki Beach Marriott | Marriott Bus Depot |
| | Hilton Waikiki Beach | Marriott Bus Depot |
| | Convention Center | Front of Convention Center |
| 5 | Inter-Hotel | All Hotel Loading Areas Referenced Above |

| ROUTE | TIME | FREQUENCY |
|--|----------------------------|---------------------------------|
| DECEMBER 15 SCHEDULE | | |
| 1 2 3 4 | 7:00 AM – 9:00 AM | Every 15 Minutes |
| | 9:00 AM – 4:00 PM | Every 30 Minutes |
| | 4:00 PM – 5:30 PM | Every 15 Minutes |
| 5 | 7:00 AM – 10:30 PM | Every 15 Minutes |
| SPECIAL OPENING CEREMONY & RECEPTION SHUTTLE TO & FROM SHERATON WAIKIKI • DECEMBER 15 ONLY • 5:30 PM–10:30 PM | | |
| 1 | Hilton Hawaiian Village | Tapa Front Bus Stop |
| | Doubletree Alana | Front of hotel |
| | Ramada Plaza | Front of hotel |
| | Sheraton Waikiki | Sheraton Bus Depot |
| 3 | Hyatt Regency Waikiki | Hyatt Koa Ave Entrance |
| | Pacific Beach Hotel | Hyatt Koa Ave Entrance |
| | Sheraton Princess Kaiulani | Hyatt Koa Ave Entrance |
| 4 | Waikiki Beach Marriott | Marriott Bus Depot |
| | Hyatt Place | Marriott Bus Depot |
| | Hilton Waikiki Beach | Marriott Bus Depot |
| | Sheraton Waikiki | Sheraton Bus Depot |
| 6 | Ala Moana | Ala Moana Mahukona St. Entrance |
| | Sheraton Waikiki | Sheraton Bus Depot |

| ROUTE | TIME | FREQUENCY |
|----------------------------------|--------------------|------------------|
| DECEMBER 16 – 19 SCHEDULE | | |
| 1 2 3 4 | 7:00 AM – 9:00 AM | Every 15 Minutes |
| | 9:00 AM – 4:00 PM | Every 30 Minutes |
| | 4:00 PM – 10:00 PM | Every 15 Minutes |
| 5 | 7:00 AM – 10:00 PM | Every 15 Minutes |

| ROUTE | TIME | FREQUENCY |
|---|--------------------|------------------|
| DECEMBER 20 SCHEDULE | | |
| 1 2 3 4 | 7:00 AM – 12:00 PM | Every 15 Minutes |
| | 12:00 PM – 1:00 PM | Every 30 Minutes |
| | 1:00 PM – 4:00 PM | Every 15 Minutes |
| 5 | 7:00 AM – 12:00 PM | Every 15 Minutes |
| SPECIAL CLOSING RECEPTION SHUTTLE TO & FROM HILTON HAWAIIAN VILLAGE • DECEMBER 20 ONLY • 1:00 PM – 4:00 PM | | |



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American Chemical Society (ACS)



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Royal Australian Chemical Institute (RACI)



Korean Chemical Society (KCS)



Chinese Chemical Society (CCS)