21COE Programme: Mechanical Systems Innovation Open Seminar

21COE Programme: The Mechanical System Innovation Open Seminar 2007 will be held as follows. Professor David Tománek is well known for his pioneering molecular scale simulation works related to carbon nanotubes and other structures. He is also famous for his "The Nanotube Site," and organization works for NT0X international meetings. Participants from any departments will be welcome.

Invited Speaker : Professor David Tománek, Physics and Astronomy Department, Michigan State University

Title :

Real-time *ab initio* calculations of excited-state dynamics in carbon nanostructures

Date & Time: 22 January 2007, 13:00pm~14:30pm

Place: The University of Tokyo, Engineering Building II, 2nd Floor, Seminar Room 1

Abstract:

The quantum nature of phenomena, dominating the behavior of nanostructures such as nanotubes, raises new challenges when trying to predict and understand their response to electronic excitations. Addressing this challenge is imperative in view of the continuous reduction of device sizes, which is rapidly approaching the atomic level. Due to fundamental limitations imposed on observations by the quantum nature of these systems, *ab initio* computer simulations, involving a combination of time-dependent density functional theory for electrons and molecular dynamics for the ions, emerge as a powerful tool to understand and predict the behavior of nanotubes following electronic excitations [1].

Addressing possible limitations in the frequency response of carbon nanotube-based electronic components, I will discuss the microscopic decay mechanism of photoexcitations [2], including the cross-over from purely electronic to phonon decay channels, and show its temperature dependence, as shown in Fig. 1. Depending on the energy scale, electronic excitations may play a decisive role in determining the outcome of sputtering events by ions, which could induce selective structural modifications. Nanotubes, one of the most promising building blocks of Nanotechnology, display an unexpected defect tolerance, owing to an efficient self-healing mechanism, which may be triggered by electronic excitations [3]. Due to the long lifetime of electronic excitations in nanotubes, which is comparable to phonon periods, irradiation by monochromatic light emerges also as a selective and powerful

technique to purify nanotubes from chemical impurities [4].

References

[1] David Tománek, Carbon-based nanotechnology on a supercomputer, Topical Review, J. Phys.: Condens. Matter **17**, R413-R459 (2005).

[2] Yoshiyuki Miyamoto, Angel Rubio, and David Tománek, Real-time *ab initio* simulations of excited carrier dynamics in carbon nanotubes, Phys. Rev. Lett. **97**, 126104 (2006).

[3] Yoshiyuki Miyamoto, Savas Berber, Mina Yoon, Angel Rubio, David Tománek, Can Photo Excitations Heal Defects in Carbon Nanotubes? Chem. Phys. Lett. **392**, 209 (2004).

[4] Yoshiyuki Miyamoto, Noboru Jinbo, Hisashi Nakamura, Angel Rubio, and David Tománek, Photodesorption of oxygen from carbon nanotubes, Phys. Rev. B **70**, 233408 (2004).

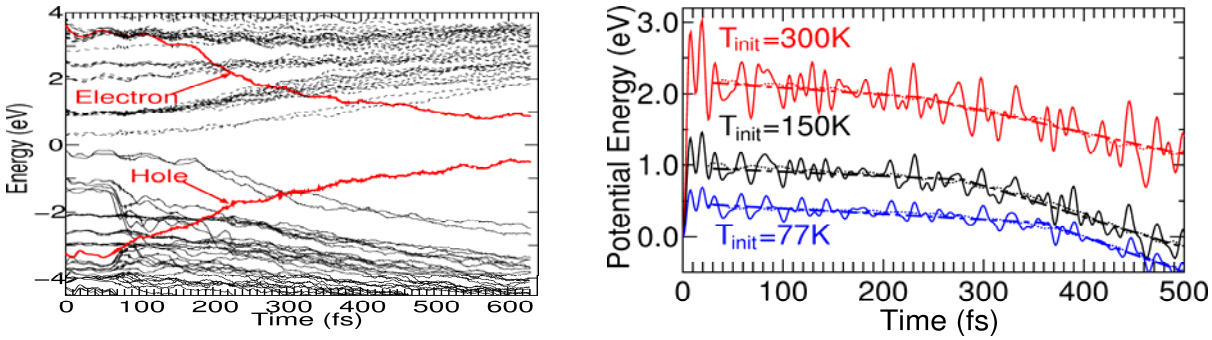

Figure 1. Left: Time-dependence of Kohn-Sham state during a decaying an electron-hole excitation in a (3,3) carbon nanotube. Right: Time dependence of the ionic potential energy in the system [2].

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