

Defect Engineering in 2-Dimensional Materials: From Theory to Applications

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This talk will first provide an overview of different defects in 2-Dimensional materials such as graphene and Chalcogenides. We will then discuss the synthesis of large-area, high-quality monolayers of nitrogen- and boron-doped graphene sheets on Cu foils using ambient-pressure chemical vapor deposition (AP-CVD). Scanning tunneling microscopy (STM) and spectroscopy (STS) reveal that the defects in the doped graphene samples arrange in different geometrical configurations exhibiting different electronic and magnetic properties. Interestingly, these doped layers could be used as efficient molecular sensors and electronic devices. In addition, the synthesis of hybrid carbon materials consisting of sandwich layers of graphene layers and carbon nanotubes by a self-assembly route will be discussed. These films are energetically stable and could well find important applications as field emission sources, catalytic supports, gas adsorption materials and super capacitors.

Beyond graphene, the synthesis of other 2-Dimensional materials will be described. In particular, we will discuss the synthesis of WS₂ and MoS₂ triangular monolayers, as well as large area films using a high temperature sulfurization of WO_x clusters deposited on insulating substrates. We will show that depending on the substrate and the sizes of the oxide clusters, various morphologies of layered dichalcogenides could be obtained. In addition, photocurrent measurements on these materials will be presented. Our results indicate that the electrical response strongly depends on the laser photon energy. The excellent response observed to detect different photon wavelengths in MoS₂, WS₂ and WSe₂ materials, suggest these materials could be used in the fabrication of novel ultrafast photo sensors.

From the theoretical stand point, we have found using first principles calculations, that by alternating individual layers of different metal chalcogenides (e.g. MoS₂, WS₂, WSe₂ and MoSe₂) with particular stackings, it is possible to generate direct band gap bi-layers ranging from 0.79 eV to 1.157 eV. Interestingly, in this direct band gap, electrons and holes are physically separated and localized in different layers. We foresee that the alternation of different chalcogenide layers would result in the fabrication of materials with unprecedented optical and physico-chemical properties.

Mauricio Terrones, obtained his B.Sc. degree in Engineering Physics with first class honors at Universidad Iberoamericana, and was distinguished as the Best Student of Mexico in Engineering Physics in 1992. In 1994 he started his doctorate degree with Sir Prof. Harold W. Kroto (Nobel Laureate, FRS), and received his D.Phil. degree from University of Sussex in 1998. He has co-authored more than 300 publications in international journals, and counts with more than 25,000 citations to his work (His H index is 79; Google Scholar H=85). He has published in *Nature*, *Science*, *Phys. Rev. Lett.*, *Nano Lett.*, *Nature Nanotechnology*, *Nature Materials*, *Nature Communications*, *ACS Nano*, etc. In 1999, he was awarded the Alexander von Humboldt Fellowship, and carried out research at the Max-Planck Institut für Metallforschung (Stuttgart, Germany). In 2000, he was recipient of the Mexican National Prize for Chemistry. He also received the Javed Husain Prize and the Albert Einstein medal from UNESCO in 2001. In 2005, he received the TWAS Prize in Engineering Physics for his contributions in the field of carbon-based nanomaterials. This prize is given by the Academy of Sciences of the Developing world, and Mauricio is the youngest scientist ever to receive any TWAS award. In 2005, Terrones also received the "José Antonio Villaseñor y Sánchez" Prize, awarded by the governor of the state of San Luis Potosí, for his contributions to Nanoscience. He is member of the Mexican Academy of Sciences since 2002. In 2007, Terrones was elected the National Contact Point in Nanotechnology with the European Union. In 2012 was elected fellow of the American Association for the Advancement of Science (AAAS). Mauricio is also Associate Editor of *Carbon*, *Journal of Materials Research* and *Nature Scientific Reports*. Aged 45, he is Professor of Physics, Chemistry and Materials Science &



Engineering with tenure at Penn State University. He is also the Founder Director of the Center for 2-Dimensional and Layered Materials at Penn State.