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

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The impact of newly developed nano-materials and nanotechnology in Engineering and Agricultural field is much anticipated. In order to propose public policy for nanotechnology-based innovative agriculture, understandings of current trend of nano-materials are essential. In this seminar, the most up-to-date nano-material, 2-dimensional materials such as graphene and chalcogenides will be discussed. 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.

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