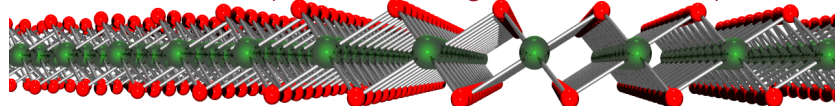




Center for the Computational Design of Functional Layered



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## **Defect Engineering in 2-Dimensional Materials: Graphene, Doped-Graphene and Beyond**

**Mauricio Terrones**

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This talk will first provide an overview of different defects in 2-Dimensional materials including graphene and Chalcogenides. In particular, we will focus on: 1) defining the dimensionalities and atomic structures of defects; 2) pathways to generating structural defects during and after synthesis and, 3) the effects of having defects on the physico-chemical properties and applications. We will then discuss the synthesis of large-area, high-quality monolayers of nitrogen-, boron- and silicon-doped graphene sheets on Cu foils using ambient-pressure chemical vapor deposition (AP-CVD). Scanning tunneling microscopy (STM) and spectroscopy (STS) demonstrate that defects in doped graphenes arrange in different geometrical configurations exhibiting different electronic and chemical properties. Interestingly, these doped layers can be used as efficient molecular sensors and electronic devices. In this context, Graphene enhanced Raman spectroscopy will be introduced and it will be explained that by doping graphene with Nitrogen, the Fermi level ( $E_F$ ) of graphene shifts, and if this shift aligns with the lower unoccupied molecular orbital (LUMO) of a molecule, charge transfer would be enhanced, thus significantly amplifying the molecule's vibrational Raman modes. Concentrations as low as  $10^{-11}$  mol/L of different dye molecules can be detected using GERS. Finally, we will discuss the controlled synthesis and assembly of chalcogenide monolayers on different substrates. The electronic performance of monolayers of  $\text{MoS}_2$ ,  $\text{WS}_2$  and hetero-systems operating under flexural strain will also be presented. Our findings demonstrate that it is now possible to use chalcogenide layers for the fabrication of flexible electronic devices, however, defect control is required to tailor their performance.

Keywords: graphene, dopant, defects

**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 400 publications in international journals, and counts with more than 31,000 citations to his work (His H index is 84; Google Scholar H=95). He has published in *Nature*, *Science*, *Phys. Rev. Lett.*, *Nano Lett.*, *Nature Nanotechnology*, *Nature Materials*, *Nature Communications*, *Nature Chemistry*, *ACS Nano*, *PNAS*, 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). In 2015, he was elected fellow of the Royal Society of Chemistry (UK) and was awarded the Jubilee Professorship from Chalmers University of Technology (Sweden). In 2016, Mauricio was awarded the Faculty Scholar Medal in Physical Sciences (Penn State). Mauricio is also Associate Editor of *Carbon*, *2D Materials*, *Journal of Materials Research* and *Nature Scientific Reports*. 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, and also the NSF-IUCRC Center for Atomically Thin Multifunctional Coatings (ATOMIC).

