Defects in 2D Metal Dichalcogenides: Doping, Alloys, Interfaces, Vacancies and Their Effects in Electronics, Catalysis, Optical Emission and Bio-Applications

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Semiconducting two-dimensional transition metal dichalcogenides (TMDs) such as MoS2, MoSe2, WSe2, and WS2 hold great promise for many novel applications. Recent years have therefore witnessed tremendous efforts on large scale manufacturing of these 2D crystals. A long-standing puzzle in the field is the effect of different types of defects in their electronic, magnetic, catalytic and optical properties.

In this presentation an overview of different defects in transmission metal di-chalcogenides (TMDs) will be presented. We will define the dimensionalities and different atomic structures of defects, and discuss how these defects could be imaged with novel optical-driven techniques. We will emphasize doping and alloying in monolayers of MoS2 and WS2, and describe their implications in electronic and thermal transport. We will also describe the catalytic effects of edges, vacancies and local strain observed in MoxW(1-x)S2 monolayers by correlating the hydrogen evolution reaction (HER) with aberration corrected scanning transmission electron microscopy (AC-HRSTEM). Our findings demonstrates that it is now possible to use chalcogenide layers for the fabrication of more effective catalytic substrates, however, defect control is required to tailor their performance. By studying photoluminescence spectra, atomic structure imaging, and band structure calculations, we also demonstrate that the most dominating synthetic defect—sulfur monovacancies in TMDs, is responsible for a new low temperature excitonic transition peak in photoluminescence 300 meV away from the neutral exciton emission. We further show that these neutral excitons bind to sulfur mono-vacancies at low temperature, and the recombination of bound excitons provides a unique spectroscopic signature of sulfur mono-vacancies. However, at room temperature, this unique spectroscopic signature completely disappears due to thermal dissociation of bound excitons. One-dimensional hetero-interfaces in TMDs will be shown by AC-HRSTEM in conjunction with their non-linear optical emission, constituting a new way to image 1D defects. Finally, the electronic effects of C-H defects within TMDs will be discussed, as p-type doping could be controlled by the presence of C within TMDs.

Dr. Terrones is Verne M. Willaman Professor of Physics and Distinguished Professor of Physics, Chemistry and Materials Science & Engineering 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). He 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 550 publications in international journals, and counts with more than 50,000 citations to his work (His H index is 104; Google Scholar H=115). Dr. Terrones is the recipient of numerous prestigious awards, including the Alexander von Humboldt Fellowship (1999), the Mexican National Prize for Chemistry (2000), the Javed Husain Prize and the Albert Einstein medal from UNESCO (2001), the TWAS Prize in Engineering Physics (2005), and the “José Antonio Villaseñor y Sánchez” Prize (2005), the Jubilee Professorship from Chalmers University of Technology (Sweden, 2005), and the Faculty Scholar Medal in Physical Sciences (Penn State 2016). He is member of the Mexican Academy of Sciences, fellow of the American Association for the Advancement of Science (AAAS), fellow of the Royal Society of Chemistry (UK), fellow of the American Physical Society (APS). Mauricio is the Editor in Chief of the journal Carbon, and he is currently associate editor of 2D Materials and Nature Scientific Reports.