Defects in 2D Metal Dichalcogenides: Doping, Alloys, Vacancies and Their Effects in Magnetism, 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 [1,2]. 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, WS2, and WSe2 and describe their implications in magnetism, as well as in electronic transport [3]. 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) [4]. 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 [5]. 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 [5]. However, at room temperature, this unique spectroscopic signature completely disappears due to thermal dissociation of bound excitons [5]. 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 [6]. 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 [7].

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