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A review of Defects in 2D Metal Dichalcogenides: Doping, Alloys, Interfaces, Vacancies and Their Effects in Catalysis & Optical Emission

In this presentation an overview of different defects in transmission metal di-chalcogenides (TMDs) will be presented [1,2]. We will first focus on: 1) defining the dimensionalities and atomic structures of defects (Fig. 1); 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 also emphasize doping and allowing monolayers of MoS_2 and WS_2, and their implications in electronic and thermal transport. We will also describe the catalytic effects of edges, vacancies and local strain observed in $Mo_xW_{(1-x)}S_2$ monolayers by correlating the hydrogen evolution reaction (HER) with aberration corrected scanning transmission electron microscopy (AC-HRSTEM) [3]. 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 [4]. 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 [4]. However, at room temperature, this unique spectroscopic signature completely disappears due to thermal dissociation of bound excitons [4]. Finally, hetero-interfaces in TMDs, will be studied and discussed by AC-HRSTEM and optical emission.

References

[1] Z. Lin, M. Terrones, et al. “Defect engineering of two-dimensional transition metal dichalcogenides”. 2D Materials 3 (2016) 022002.
[2] R. Lv, M. Terrones, et al. "Two-dimensional transition metal dichalcogenides: Clusters, ribbons, sheets and more". Nano Today 10 (2015) 559-592.
[3] Y. Lei, M. Terrones, et al. "Low temperature synthesis of heterostructures of transition metal dichalcogenide alloys (WxMo1-xS2) and graphene with superior catalytic performance for hydrogen evolution". ACS Nano, 11 (2017), 5103-5112.
[4] V. Carozo, M. Terrones, et al. “Optical identification of sulfur vacancies: Bound excitons at the edges of monolayer tungsten disulfide”, Sci. Adv. 3 (2017), e1602813.

Figures

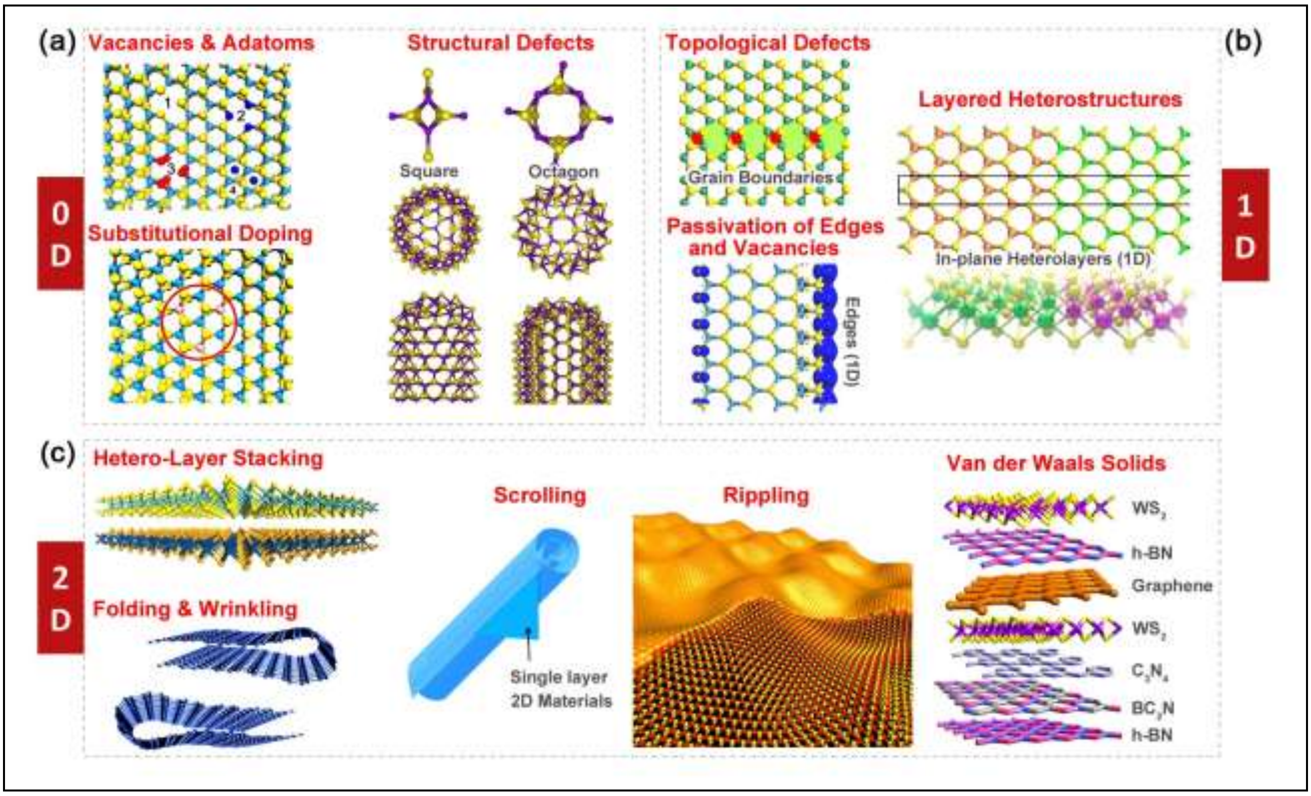

Figure 1: Different categories of defects in transition metal dichalcogenides according to their dimensionality.

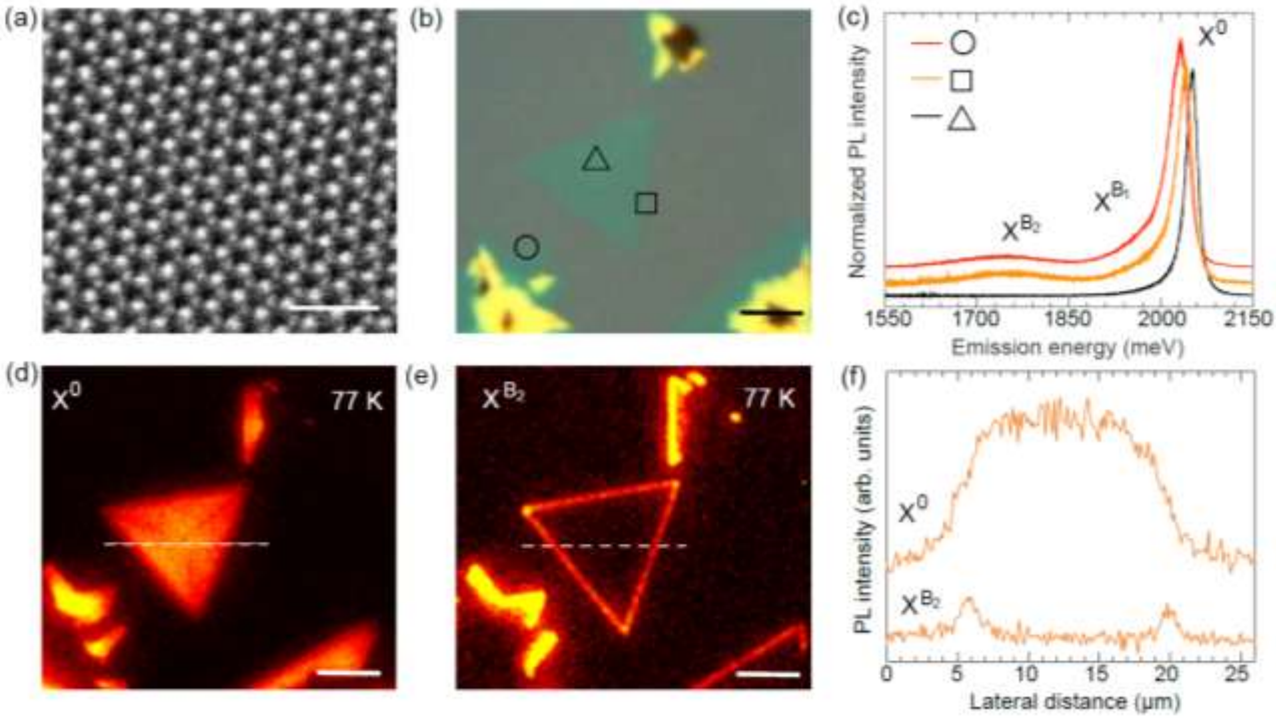

Figure 2: (a) Atomic structure of single layer 1H-WS_2. (b) Optical image of triangular WS_2. (c) PL spectra obtained from the marked regions in (b). Photoluminescence intensity image at 77 K of (d) X^0 peak centered at 1970 meV and (e) X^B peak centered at 1690 meV. (f) X^B and X^B intensity profile acquired along the dashed line in (d) and (e).