Defects in Metal Dichalcogenides: Effects in Catalysis & Optical Emission

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We will first focus on: *1)* defining the dimensionalities and atomic structures of defects [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 [2-4]. 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). Our findings demonstrates that it is now possible to use chalcogenide layers for the fabrication of more effective catalytic substrates [3], 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 [4].Finally, hetero-interfaces in TMDs, will be studied and discussed by AC-HRSTEM and optical emission.

References

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[3] Y. Lei, M. Terrones, *et al. ACS Nano*, **11** (2017), 5103-5112.
[4] V. Carozo, M. Terrones, *et al. Sci. Adv*. **3** (2017), e1602813

Figures

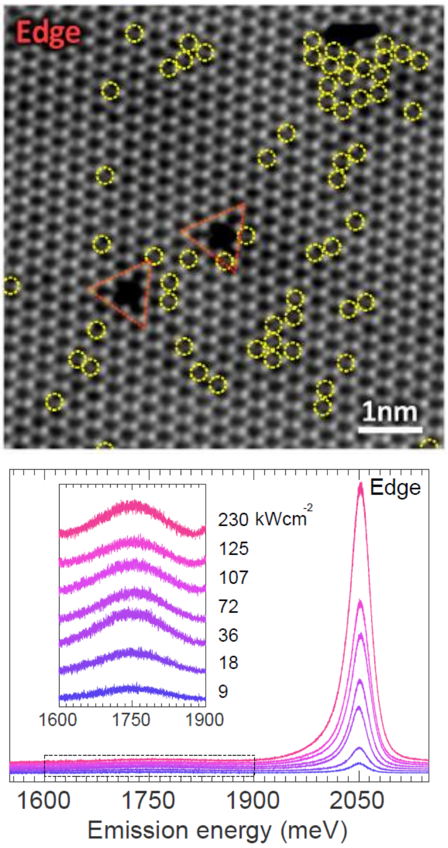

Figure 1: Top. AC-HRSTEM image of the edge of a WS_2 triangular monolayer showing more vacancies at the edges. Bottom. Evolution of the PL spectra at the edges of a triangular WS_2 monolayer with high concentrations of sulphur mono vacancies at the edges.