Chemical Passivation in 2D Semiconducting Material for Sustainable Optoelectronic Applications

Zhaojun Li
Uppsala University, Ångströmlaboratoriet, Lägerhyddsvägen 1, Uppsala, Sweden
Zhaojun.li@angstrom.uu.se

Abstract
The discovery of 2D materials based on transition metal dichalcogenides (TMDs), has opened up new interesting possibilities in optoelectronic devices, as monolayer TMDs possess direct bandgaps with absorption in the visible to near-infrared (NIR) spectral region. However, monolayer TMDs often exhibit poor photoluminescence quantum yields (PLQEs) and mobilities, which are signs of poor-quality semiconductor material. While there have been advances in materials growth in the past years, our understating of defects and how they degrade performance is still unsatisfactory. Thus, while many defect passivation strategies have been discussed in the literatures, most achieve only moderate PL enhancement. No chemical treatment has yet been able to significantly enhance both the PL and electrical mobility of 2D TMDs.[1]

Here, I will present new chemical functionalization approaches to greatly enhance the PL intensity of mechanically exfoliated monolayer molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2), while simultaneously enhancing the charge and exciton transport properties.[2,3] We propose an atomic-level synergistic defect passivation mechanism of both neutral and charged sulfur vacancies (SVs), supported by ultrafast transient absorption spectroscopy (TA), Hard X-ray photoelectron spectroscopy (HAXPES), and density functional theory (DFT) calculations. In addition, these non-corrosive chemicals are stable and operate in benign solvents under ambient conditions, making them sustainable and suitable for direct use during device fabrication of TMDs. Our findings establish a new performance benchmark for the optical and electronic properties of WS_2 monolayers, paving the way for developing sustainable 2D semiconductor technologies.

References

[1] Li, Z. *et al.* Nanoscale, 16 (2024) 9728.
[2] Li, Z. *et al.* Nat. Commun., 12 (2021) 6044.
[3] Li, Z. *et al.* J. Am. Chem. Soc.,146 (2024) 35146.

Figures

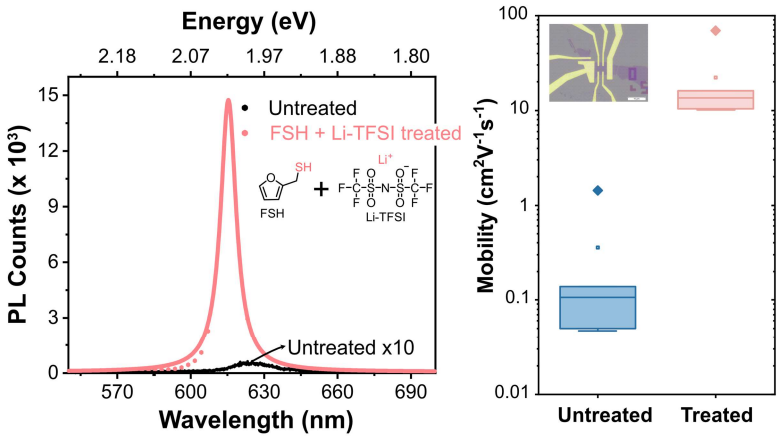

Figure 1: Sequence-Specific Chemical Passivation.