Mechanistic Insight to the Chemical Treatments of Monolayer Transition Metal Disulfides for Photoluminescence Enhancement

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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 surface passivation by chemical treatment of TMDs has been explored by several groups, thus far only a few methods have been shown to improve a few, but not all of the semiconducting properties. For instance, the use of the 'super-acid treatment' with trifluoromethanesulfonimide (H-TFSI) improves PLQE greatly but gives rise to considerable exciton and charge trapping. At the basis, the chemical mechanisms behind such passivation schemes is unclear, allowing little room for their optimisation and the generation of high-quality materials. Here, I will present new chemical functionalization approaches to greatly enhance the PL intensity of mechanically exfoliated monolayer molybdenum disulphide (MoS_2) and tungsten disulphide (WS_2), while simultaneously enhancing the charge and exciton transport properties.[1] I will also illustrate an unprecedented, detailed understanding of the passivation mechanisms. In addition, I will present a family of ionic salts with superior PL enhancement effect compared to widely discussed "super acid" H-TFSI treatment.[2] More importantly, the ionic salts used in chemical treatments are compatible with a range of greener solvents and are easier to handle compared to super acid, which provides the possibility of directly treating TMDs for device fabrication.

REFERENCES

[1] Bretscher, Hope, *et al.* ACS Nano, 15 (2021), 8780-8789
[2] Li, Zhaojun, *et al.* Nat. Commun. In press. Preprint: arXiv: 2002.03956 (2020)

FIGURES

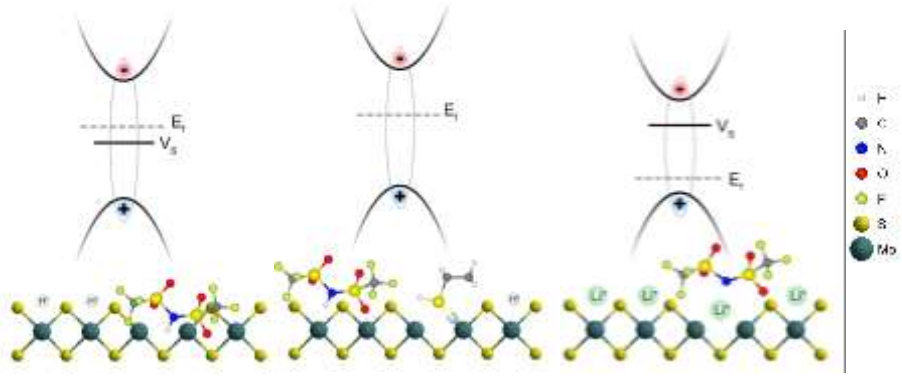

Figure 1: Schematic illustration of different chemical treatments on MoS_2.