Defect Engineering in Transition Metal Dichalcogenides (TMDs) for Optoelectronic Application

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Abstract

Two-dimensional transition metal dichalcogenides (2D-TMDs), such as WS_2 and WSe_2, exhibit great potential in optoelectronic applications due to their unique direct bandgap and high carrier mobility[1,2]. However, the presence of chalcogen vacancies introduces deep trap states, leading to severe non-radiative recombination and significantly suppressing photoluminescence (PL), posing a critical bottleneck for their practical application[3].

To address this challenge, we systematically investigated the defect behavior in monolayer WS_2 and WSe_2 by integrating multiscale characterization and theoretical calculations. Utilizing a surface chemical engineering approach, we employed Li-TFSI surface treatment, achieving effective passivation of sulfur vacancies (SVs) in both WS_2 and WSe_2. We propose an atomic-level synergistic defect passivation mechanism for both neutral and charged SVs, supported by ultrafast transient absorption spectroscopy (TA), Hard X-ray photoelectron spectroscopy (HAXPES), and density functional theory (DFT) calculations. Experimental results reveal a 250-fold PL enhancement in monolayer WS_2 and a 4-fold increase in monolayer WSe_2 after treatment[4].

While our study provides an initial understanding of defect passivation mechanisms, further atomic-scale characterizations and more universal passivation strategies are still needed to deepen our knowledge and broaden the applicability of this approach.

References

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