Mechanism of Oleic Acid-Mediated Sulfur Vacancy Healing in monolayer WS_2

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Within the group of 2D materials tungsten disulfide (WS_2) stands out due to its high photoluminescence (PL) yield. Central to the advancement of WS_2-based technologies is the precise control and manipulation of defects, with vacancies playing a crucial role.
Recently, defect healing through chemical treatments has been spotlighted as a promising method to effectively enhance PL intensity. Among various chemical agents, oleic acid (OA) has garnered significant interest due to its efficacy in increasing PL properties of WS_2 while simultaneously maintaining its doping characteristics [1]. Nevertheless, the specific mechanism underlying these observations remains unclear.
In our recent study, we propose a novel mechanism where OA counteracts the sulfur vacancy in WS_2, contributing substitutional oxygen. Through thermal treatment, we induce sulfur vacancies in WS_2, and investigate the resulting decrease in PL yield and the shift in the emission spectrum, which is later revived by treatment with OA. Interestingly, our treatment does not improve the PL yield for samples free of vacancies on the surface or containing other defect types.
Using density functional theory calculations, we provide insight into the underlying mechanism governing the oleic acid-mediated sulfur vacancy healing process.
Our research suggests that proficient defect passivation through oxygen doping can be successfully achieved using chemical treatment, thus laying down a foundational pathway for oxygen doping in TMDCs. However, we also highlight the limitations of chemical treatment, which may only lead to small increases in photoluminescence yield beyond a certain point.

References

[1] Arelo O. A Tanoh *et al.,* Nano Letters, 19, 9 (2019) 6299–6307

Figures