Impact of Sulfur Vacancy on Confined Water Between SiO_2 and WS_2

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Transition metal dichalcogenides (TMDs) are studied extensively in electronic devices due to their 2D nature and semiconducting properties. Typically, films are transferred by mechanical exfoliation onto substrates, such as the industry standard SiO_2. However, the influence of the substrate on film properties remains an understudied area. Notably, water layers atop SiO_2 under ambient conditions add intricacy to the interface between TMDs and the substrate. Moreover, the prevalence of sulfur vacancies on the basal plane of TMDs introduces complexities, potentially initiating the oxidation process of the TMD. [1-3]

In this work, we investigate the SiO_2/WS_2 interface, exploring the impact of varying thicknesses of water confined between these materials utilizing Density Functional Theory (DFT), Classical Molecular Dynamics (MD), and Ab Initio Molecular Dynamics (AIMD). Pristine and defective interfaces were constructed to understand the geometry and electronic properties differences. Our work found that introducing a sulfur vacancy induces restructuring of confined water, drawing it closer to the WS_2 surface. This alteration also prompts charge redistribution at the interface. Our findings suggest that the sulfur vacancy intensifies water interaction with WS_2, highlighting its pivotal role as a potential site for oxidation.

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