Impact of interface and surface oxide defects on WS_2 electronic properties from first-principles

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From an industrial point-of-view, the scalable growth of an oxide on top of a 2D channel without degrading its transport properties remains a challenge nowadays [1]. In this work, we construct several interface models between amorphous (am-) Al_2O_3/HfO_2 and a WS_2 monolayer (see Fig.1) in order to investigate their impact on the 2D properties using first-principles. We show that, while it is in principle possible to achieve a van der Waals (vdW) interface between those materials, surface defects (e.g., undercoordinated metal atoms) are detrimental to transport since they create localized states close to the bottom of the conduction band of WS_2. Even in the perfect case scenario, the inhomogeneity of the surface creates a non-uniform potential felt by charge carriers in WS_2 (see Fig.2), similarly to what has been suggested in Ref. [2]. While the surface defects can potentially be kept under control with an appropriate choice of the top oxide, the surface inhomogeneity shall ultimately be the bottleneck for the oxide growth on top of WS_2 by atomic layer deposition.

References

[1] K. P. O'Brien, *et al.*, Nature Communications 14 (2023) 6400
[2] A. Raja *et al.*, Nature Nanotechnology 14 (2019) 832–837

Figures

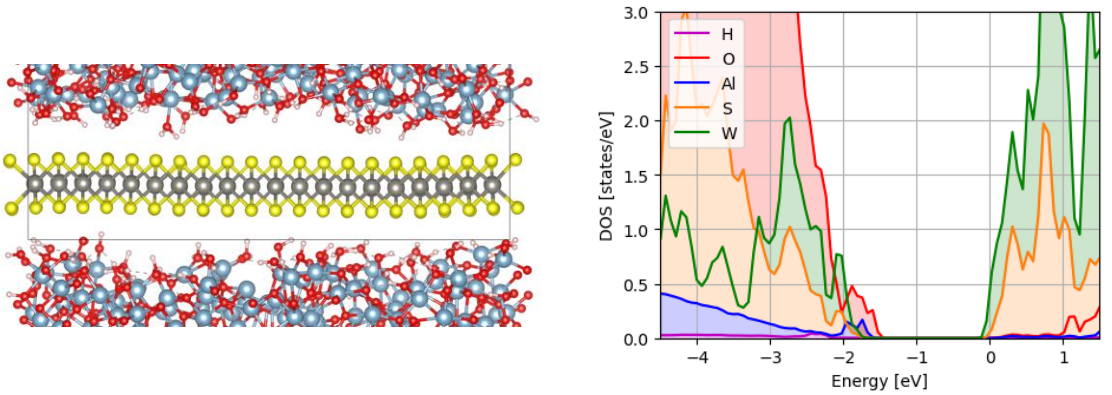

Figure 1: Atomistic view of vdW interface between WS_2 and am-Al_2O_3 and corresponding PDOS.

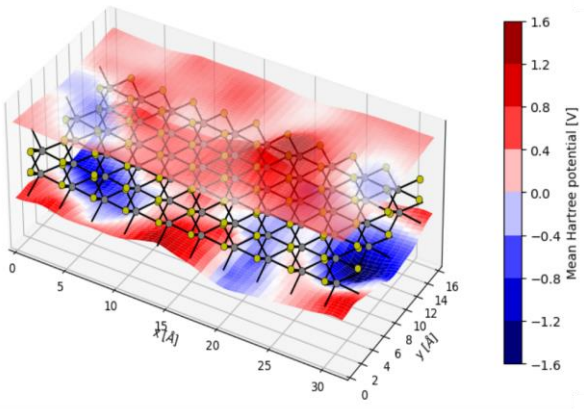

Figure 2: Average Hartree potential felt by an electron in WS_2 due to the presence of the oxide.