# Oxide induced degradation in $MoS_2$ Field-Effect Transistors

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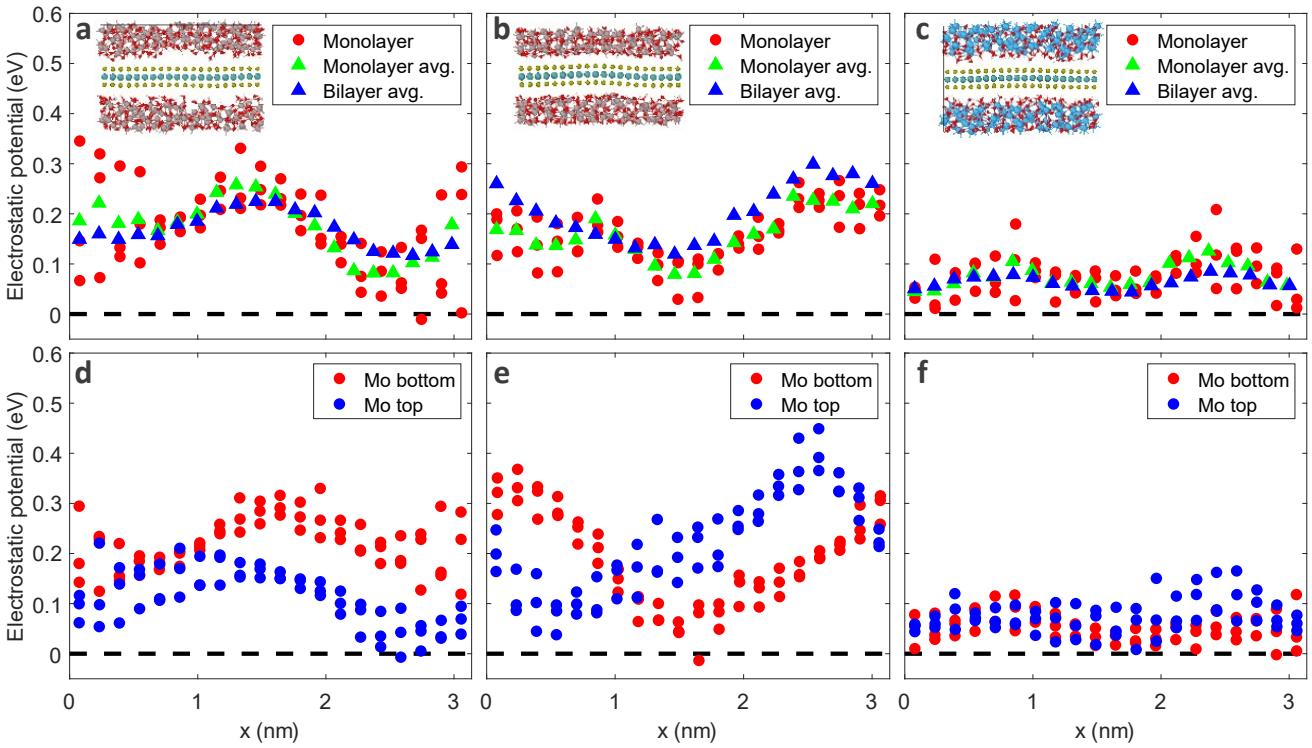


Figure 1: Potential fluctuations induced by the models M1 to M3 in mono- (a) to (c) and bilayer (d) to (f) $MoS_2$. The red dots in (a) to (c) denote the electrostatic potential of each Mo atom. The green and blue triangles show the electrostatic potential averaged over the width of the unit cell and the layers for mono- and bilayers, respectively. Additionally, the inset presents a visualization of the models M1 to M3. (d) to (f) report the electrostatic potential of the top (blue) and bottom (red) layer of bilayer $MoS_2$. M1 and M2 feature am-$Al_2O_3$, while M3 has am-$HfO_2$.

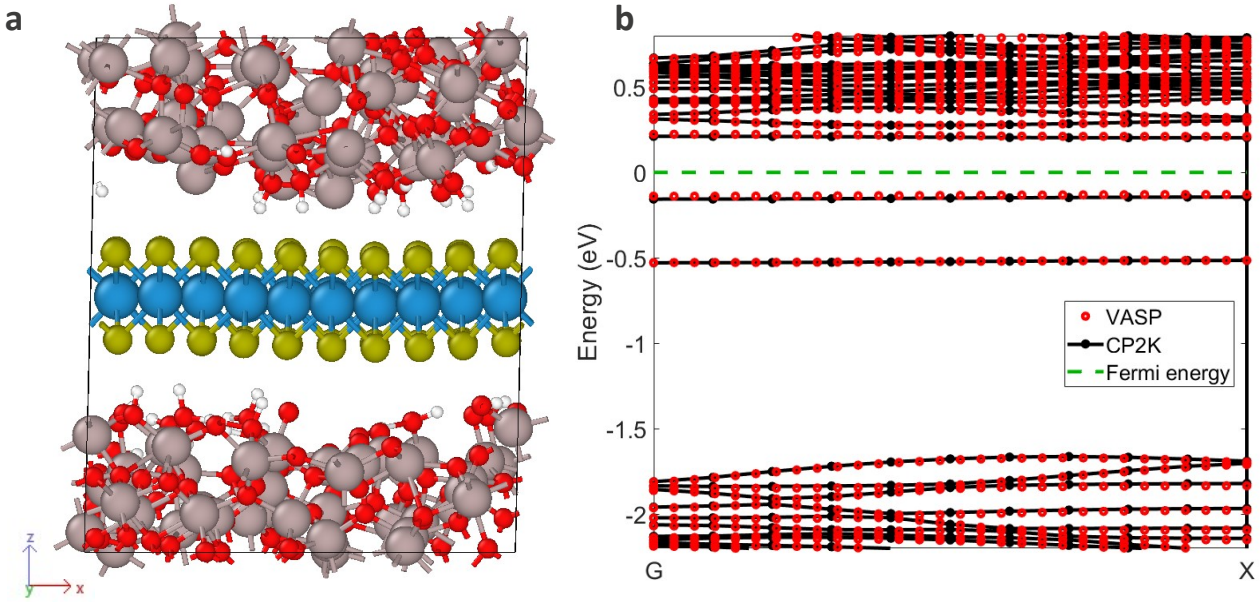


Figure 2: Comparison between VASP and CP2K. (a) Atomic configuration of the test structure with $WS_2$/am-$Al_2O_3$. It contains 30 and 60 W (blue) and S (yellow) atoms, respectively, as well as 100, 165, and 36 Al (gray), O (red), and H (white) atoms. (b) Band structure of the unit cell (a) in x-direction. The black and red dots denote the CP2K and VASP eigenvalues while the black lines serve to guide the eye. With CP2K we employed a Gaussian Type Orbital (GTO) basis set of double-zeta valence (DZVP). Except on W, where a triple-zeta valence (TZVP) basis was used. This combination leads to an excellent agreement with the plane-wave basis of VASP.