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First Principles Study of Electronic Properties of MoS_2/HfO_2 Interface[1] SANTOSH KC, ROBERTO C. LONGO, ROBERT M. WALLACE, KYEONGJAE CHO, Univ of Texas, Dallas — Monolayer MoS_2 is direct band gap two dimensional (2D) semiconductor which has been recently investigated for low-powered field effect transistors and shown promising performance of high on/off current ratio (10^8) and a carrier mobility $\sim$ 200 cm^2/Vs with a high-k gate dielectric [1]. For a detailed understanding of the MoS_2 electronic devices, it is important to examine the detailed atomic and electronic structures of the MoS_2/HfO_2 interface. We have developed a lattice matched MoS_2/HfO_2 interface model, and investigated the interface atomic structures and the corresponding electronic structures using the density functional theory (DFT) calculations. The model interface was extensively investigated as a function of oxygen and hydrogen incorporation representing different HfO_2 growth conditions on MoS_2. The interface formation energies show strong effects of interfacial oxygen content and the valence band offset. *In situ* XPS study of HfO_2 ALD on MoS_2 shows that the experimental MoS_2/HfO_2 interface properties are consistent with DFT results [2]. These studies can be extended to other TMDs in an effort to identify most promising candidates for electronic device applications.

[1] B. Radisavljevic *et.*al, *Nat. Nanotechnol.* **6**, 147 (2011).
[2] S. McDonnell *et.* al. *ACS Nano* (Just Accepted).

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