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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.


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