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Ab initio Study of Metal Interfaces with HfO_2 and SiO_2: Work Function Modulation BLANKA MAGYARI-KÖPE, YOSHIO NISHI, Electrical Engineering, Stanford University, CA, LUIGI COLOMBO, Texas Instruments Incorporated, Dallas, TX, KYEONGJAE CHO, Physics and Electrical Engineering, University of Texas, Dallas, TX — For the next generation of metal-oxide-semiconductor field-effect transistors (MOSFETs), the suitable metal candidate has to be identified. The choice of a specific metal electrode on high-k gate dielectric oxide films is strongly influenced by the possible interface chemical reactions and defects. In this study, *ab initio* calculations are employed to investigate and analyze a number of possible interface structures between gate dielectric oxides, HfO_2 and SiO_2, and metal electrodes. The structural stability and electronic structure of the interfaces with implications to metal work functions are discussed. The work function of metals on oxides is significantly influenced by the interface configurations and by the particular bonding pattern at the interface. For work function modulation, model interface systems of metal bi-layers are constructed based on structural and compositional heterogeneity. It is found that a few atomic layers of the underlying metal shift the work function of bi-layers to that of underlying metal.

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