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Internal dielectric interface: SiO_2/HfO_2. ONISE SHARIA, ALEX DEMKOV, GENADI BERSUKER, BYOUNG HUN LEE — We investigate theoretically the atomic structure of the SiO_2-HfO_2 interface, its energretics, and thermodynamic stability with respect to oxygen exchange across the interface. We have examined the electronic properties of the interface including the band discontinuity. All calculations are performed using density functional theory. We employ ultrasoft pseudopotentials, and a plane wave basis set. To model the interface we build a supercell structure by connecting β-crystobalite (crystalline silica polymorph) and cubic hafnia. This model, while being obviously rather simplistic allows for systematic study of the dielectric thickness effects, and consistent placement of defects with respect to the interface. We use the idealized C9 structure of crystobalite (silica is assumed to be relaxed). The hafnia cell is matched to crystobalite *via* a 45 $^{\circ}$ rotation and is assumed to be under the 4% tensile strain. Wee allow for the elongation of the c axis in response to strain. The striking atomic feature of the calculated interface structure is three-fold coordinated interfacial oxygen atoms connected to one Si and two Hf neighbors. The Si-O and Hf-O bond lengths are 1.62 and 2.1 Å, respectively. The energy of the interface is estimated to be in the range of 900-4000 erg/cm^2 depending on the oxygen chemical potential. The structure has no states in the gap. We then consider the relative energies of oxygen vacancies on both sides of the interface. We investigate different positions and different charge states of the vacancy.

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