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Ab initio study of the epitaxial ZrO2/Si interface[1] MEHMET DOGAN, DIVINE KUMAH, CHARLES AHN, FREDERICK WALKER, SOHRAB ISMAIL-BEIGI, Yale University — Growing thin films of crystalline metal oxides on semiconductors has been of much scientific interest because of the potential applications of such systems in electronic devices. One particular research goal is to achieve ferroelectricity in a crystalline and thin oxide film that is epitaxial on a semiconductor. This would enable one to realize non-volatile field-effect transistors where the state of the system is encoded in the polarization direction of the oxide. In this work, we study oxides that are not ferroelectric in the bulk but become ferroelectric as an ultrathin film on a semiconductor such as silicon. Recent developments in epitaxial growth methods also permit fabrication of such systems. Here, we use density functional theory to study the interface between ZrO_2 and Si. When the oxide is only 1 monolayer thick, we find a set of stable structures with a variety of positive and negative out-of-plane ferroelectric polarizations. We present an analysis of these structures as a function of oxide thickness and the size of interface unit cell. Furthermore, the ZrO_2 can be used as a buffer layer to induce ferroelectricity in ultrathin perovskite oxides such as $SrTiO_3$ on Si which can couple the oxide polarization to the silicon carrier density.

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