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Ab initio study of ZrO2 monolayers epitaxial on Si[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 their applications in electronic devices. One research goal is to achieve ferroelectricity in a crystalline and thin oxide film that is epitaxial on a semiconductor. This would enable the realization of non-volatile field-effect transistors where the state is encoded in the polarization direction of the oxide. We study oxides that are not ferroelectric in the bulk but become ferroelectric as an ultra-thin film on a semiconductor. Recent advances in epitaxial growth methods permit fabrication of such systems. We use density functional theory to study the interface between ZrO_2 monolayers and Si (001). These monolayers have multiple metastable states. We present an analysis of these configurations and energy barriers between them. We consider the likely experimental situation where different configurations coexist to form a multi-domain system, and investigate domain dynamics. Furthermore, we demonstrate that the ZrO_2 monolayers can be used as a buffer layer to induce ferroelectricity in perovskite oxides such as $SrTiO_3$ on Si. We also show that these monolayers modify the transport properties of Si which would allow for the desired device applications.

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