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Interfacial effects on ferroelectricity in $SrTiO_3$ thin films supported on Si(001) ALEXIE KOLPAK, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena (CRISP) and Department of Applied Physics, Yale University, New Haven, CT 06520 — Experimental and theoretical studies have suggested that the application of a compressive in-plane strain can induce a polar ground state in thin $SrTiO_3$ films. One way to impose such a strain is to grow the film epitaxially on a lattice mis-matched substrate. However, it is unclear whether such films are ferroelectric – i.e., switchable – in addition to being polar, and furthermore, what role the substrate plays in determining the switchability. Using density functional theory, we explore the possibility of a ferroelectric ground state in $SrTiO_3$ thin films grown on a Si(001) substrate. In particular, we examine the effects of several proposed interface structures on the interfacial charge compensation and polarization direction, and we discuss the implications of these effects for potential applications in integrated electronics devices.

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