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First-principles-based modeling of epitaxial-strain-induced ferroelectricity in $CaTiO_3$ QIBIN ZHOU, KARIN RABE, Rutgers University — Epitaxial strain can be used to induce phase transitions from the bulk phase to non-bulk phases in thin films and superlattices. In $CaTiO_3$, it has been previously shown that tensile epitaxial strain induces a transition from the nonpolar bulk orthorhombic phase to a ferroelectric phase. In this study, our first-principles computations revealed that compressive strain also induces ferroelectric phases, one of which has unexpected in-plane polarization. To construct a parametrized energy function that reproduces the properties of $CaTiO_3$ for epitaxial strain over a wide range, I developed an approach in which the parameters in a symmetry expansion are determined by a combination of curve-fitting and constraints to computed first-principles results. This energy function allows the analysis of the competition between the oxygen-octahedron-rotation distortion and the polar mode. The use of this function in modeling the structures and properties of superlattices containing $CaTiO_3$, and in constructing effective Hamiltonian for large scale studies, will be discussed.

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