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First-Principles Study of Lattice Instabilities in the Ca-Ti-O Layered Perovskites NICOLE BENEDEK, Cornell Center for Materials Research, Cornell University, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University — Advances in complex oxide thin-film growth techniques have allowed researchers to grow materials under a wide range of epitaxial strains. It is now possible to tune the properties of oxides (the paraelectric-to-ferroelectric transition temperature, for example) simply by choosing an appropriate substrate. Another path towards tailoring properties at the atomic scale is the controlled alteration of a material's structure via two-dimensional layering. We use first-principles Density Functional Theory (DFT) to study lattice instabilities in a family of Ca-Ti-O layered perovskites. We use symmetry arguments, in combination with DFT results, to analyze the interaction between polar and non-polar lattice modes in a homologous series of Ca-Ti-O layered materials. Our results may lead to an understanding of the emergence of a novel polar state in the more general family of ferroelectric heterostructures.

Nicole Benedek
Cornell University

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