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Ferroelectrics with a trilinear coupling of three lattice modes: Response to electrical boundary conditions from first principles ANDREW T. MULDER, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Recent progress in the design of functional materials has led to the discovery of several ferroelectrics with the polarization coupled trilinearly to two nonpolar lattice modes. Because nonpolar lattice modes in perovskites play a key role in determining electronic and magnetic properties, these materials have a polarization that is strongly coupled to other functionality by design. But many properties of trilinear ferroelectrics remain unknown, and general design rules have been difficult to uncover. For example, the electrical properties are unclear because trilinear ferroelectrics may have a conventional ferroelectric mechanism, or may not (like an improper ferroelectric). Understanding the polarization response to electrical boundary conditions is therefore an open question that will impact the application of trilinear ferroelectrics to practical devices. In this talk, we use first principles methods to study the single domain polarization response to changing electrical boundary conditions in a variety of trilinear ferroelectrics. We clarify the design rules, the connection to phenomenological models (proper, improper, and weak ferroelectricity), and we show how epitaxial strain can tune a single trilinear ferroelectric between proper and improper ferroelectricity.

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