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Accessing hidden isosymmetric phase transitions in perovskite thin films JAMES RONDINELLI, Argonne National Laboratory, SINISA COH, Rutgers University — Isosymmetric phase transitions (IPT), which show no change in occupied Wyckoff positions or crystallographic space group, are exceedingly rare in crystalline matter because most condensed systems respond to external stimuli by undergoing "conventional" symmetry-lowering displacive, martensitic or reconstructive transitions. In this work, we use first-principles density functional calculations to identify an elusive IPT in orthorhombic ABO_3 perovskite oxides with tendency towards rhombohedral symmetry. Using perovskite $LaGaO_3$ as our prototypical system, we show that the latent isosymmetric phase transition, which manifests as an abrupt change in the octahedral rotation axis, is accessible only with an external elastic constraint—bi-axial strain. We show the transition originates from a soft phonon that describes the geometric connectivity and relative phase of the GaO_6 polyhedra. By connecting the origin of IPT to a chemical and structural incompatibility between the lattice and the elastic constraints, we describe how subtle changes in bulk orthorhombic and monoclinic symmetries are critical to the complete engineering of structure-correlated electronic properties in thin films. Because bi-axial strain is the critical parameter controlling the IPT, we suggest heteroepitaxial synthesis of IPT materials is a plausible route to realize high-κ dielectric actuators with variable band gaps and dielectric anisotropies.

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