

Abstract Submitted
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Ferroic Coupling in Layered Perovskites from First Principles

TURAN BIROL, School of Applied and Engineering Physics, NICOLE BENEDEK, Cornell Center for Materials Research, CRAIG FENNIE, School of Applied and Engineering Physics — Antiferrodistortive SrTiO_3 can be driven ferroelectric with a modest amount of biaxial strain. The $n = 1$ Ruddlesden-Popper remains paraelectric and undistorted for the same strain state. Elucidating the manner in which ferroic instabilities emerge as the number of perovskite blocks, n , increases is a fundamentally interesting challenge in its own right, yet a proper understanding could open new avenues in materials design. Combining first-principles calculations and symmetry arguments, we study the effect of strain (or pressure) and dimensionality on ferroic coupling in the layered Sr-Ti-O perovskites.

Turan Birol
Cornell University

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