

Abstract Submitted
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Polarization rotation in epitaxially strained perovskite-oxide superlattices¹ SERGE NAKHMANSON, Argonne National Lab — Utilizing first-principles computational techniques, we have mapped out Γ -point structural instabilities in $(\text{BaTiO}_3)_8/(\text{SrTiO}_3)_4$ superlattices held at varying degrees of epitaxial strain and constrained to P4mm symmetry with fully developed polarization in the out-of-plane direction. We find that at compressive strains larger than -0.5% (with respect to a fully relaxed P4mm structure) the superlattices exhibit no structural instabilities. However, at a smaller compressive strain, an in-plane ferroelectric instability emerges in the SrTiO_3 layers. This instability is then complemented by a similar instability in the BaTiO_3 layers that develops at tensile strain of more than 0.2%, suggesting nonzero polarization components for both in- and out-of-plane directions throughout the whole superlattice.

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