

Abstract Submitted
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Probing Ferroelectricity in Thin-film Perovskite SnTiO₃ with First-principles Structural Instability Analysis¹ WILLIAM PARKER, JAMES RONDINELLI, SERGE NAKHMANSON, Argonne National Laboratory — Perovskite SnTiO₃ has been recently identified in a number of computational studies as an attractive, environmentally-friendly material with potential to replace ferroelectric PbTiO₃. However, additional computational evidence suggests that bulk perovskite SnTiO₃ may be metastable. Using density-functional theory and phonon-band instability analysis, we investigate avenues for epitaxial stabilization of ferroelectric perovskite SnTiO₃ thin films with applied strains of up to $\pm 2\%$.

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