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Epitaxial strain tuning of polarization and band gap in perovksite $SnTiO_3$[1] WILLIAM PARKER, SERGE NAKHMANSON, Argonne National Laboratory, JAMES RONDINELLI, Drexel University — Lead toxicity has motivated theoretical studies of a tin-based perovskite ferroelectric material. Density-functional calculations predict a polar perovksite ground state for $SnTiO_3$. Simulated epitaxial strain up to $\pm 2\%$ tunes both the magnitude of the polar distortion, its direction, and the electronic band gap — compressive bi-axial strain creates the largest polar distortions, which occur entirely in the growth direction, while tensile strain reorients the polar displacements, enlarging the band gap. Projected densities of states indicate that the broken four-fold symmetry of the non-growth-oriented distortion allows Ti d_{xy} bands to mix with O p_x bands, further separating the valence band maximum and conduction band minimum. Comparing Sn and Pb in the perovskite titanate phases shows similar trends and suggests that $SnTiO_3$ ferroelectrics may be viable thin-film alternatives to Pb-based oxides.

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