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First-principles study of novel routes to ferroelectricity using strain ALISON HATT, NICOLA SPALDIN, University of California, Santa Barbara — We use first-principles density functional theory (DFT) to explore the use of strain to induce ferroelectricity in otherwise non-polar materials. First, we investigate the polarization induced in $LaAlO_3$ by changing in-plane bondlengths while constraining the unit cell to tetragonal symmetry. We then relax the symmetry constraint to examine the effect of oxygen octahedra rotations on the polarization. Next we explore whether epitaxial strain in the pseudocubic [100] direction can lift the inversion center in otherwise centrosymmetric $BiMnO_3$ and induce the small polarization reported in thin films. By studying these systems with DFT calculations, we have the ability to finely vary the system constraints, predicting new functional materials and providing insight into the underlying physics.

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