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Ab Initio Study of Multiferroicity in La(Al,Fe,Cr)O_3 ALISON HATT, Physics Department, UC Santa Barbara, NICOLA SPALDIN, Materials Department, UC Santa Barbara — We present the results of *ab initio* density functional calculations of perovskite-structure La(Al,Fe,Cr)O_3. Our calculations reveal two structurally distorted ground states of opposite polarization. Motivated by the growth of three-layer superlattices with enhanced polarization, we investigate the ferroelectricity and magnetic ordering of the La(Al,Fe,Cr)O_3 system with the goal of finding emergent multiferroicity due to interfacial strain and inversion symmetry breaking. Finally, we investigate constrained tetragonal $LaAlO_3$ to determine its role in the ferroelectric properties of the supercell.

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