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First-principles determination of low-energy structures in epitaxially-strained perovskite $SrMnO_3$ JIALAN ZHANG, KARIN RABE, Rutgers, The State University of New Jersey — Using a physically-motivated form for the energy as a function of magnetic ordering and lattice distortions around the high symmetry reference structure, we present a systematic method for determining the ground state and low-energy structures of transition-metal ABO_3 compounds from first principles. The structural information obtained through this method forms the foundation for the first-principles structural determination of the structure of perovskite oxide superlattices. The method is demonstrated for $SrMnO_3$, which has a nontrivial phase sequence with varying epitaxial strain that has been of recent interest both in first-principles and experimental investigations.

Jialan Zhang
Rutgers, The State University of New Jersey

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