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Epitaxial-strain-induced multiferroicity in $SrMnO_3$ from first principles JUN HEE LEE, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University — In the first-principles search for new ferromagnetic-ferroelectric multiferroics, one key indicator is the softening of the lowest frequency polar phonon with ferromagnetic ordering from a paraelectric antiferromagnetic bulk state. In a first-principles survey of the phonon dispersions of a wide range of magnetic perovskites, we identified $SrMnO_3$ as a promising candidate system. We find that a ferromagnetic-ferroelectric phase is stabilized by both compressive and tensile epitaxial strain. For compressive strain, there is a sequence of intermediate magnetic transitions, first to C-AFM and then to A-AFM ordering, with an increasing fraction of ferromagnetically aligned nearest neighbor Mn. At each of these, the change in magnetic order is accompanied by a jump in the magnitude of the electric polarization, so, near the A-AFM-FE→FE-FM phase boundary at 3.4% and G-AFM-FE→FE-FM phase boundary at -2.9%, an applied electric field can induce a nonzero magnetization, and the jump in c-lattice constant at -2.9% strain can generate a large piezomagnetic response. The origin of the large phonon softening in $SrMnO_3$ will be examined, which should provide guidance in identifying additional candidate systems for epitaxial-strain-induced multiferroicity.

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