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**First-principles study of spin-lattice and spin-phonon couplings in $SrMnO_3/LaMnO_3$ superlattice** YUANJUN ZHOU, KARIN RABE, Rutgers University — We have studied the influence of epitaxial strain on magnetic orderings and the couplings between the spin and optical phonons in $SrMnO_3/LaMnO_3$ superlattices using first principles. We first couple octahedral rotations with structural relaxations in ferromagnetic (FM), A-type antiferromagnetic (A-AFM) and C-type AFM (C-AFM) states, and obtain the sequence of magnetic phases with epitaxial strain. We also find that oxygen octahedral rotations lower the ground state energy but do not destroy the strain induced magnetic phase transitions. Next, the zone-center phonon modes in FM, A-AFM, and C-AFM states are computed using the frozen phonon method. A substantial increase of the coupling strength between the spin and the lowest polar mode is observed for tensile strains. From the analysis of the eigenvectors, the effect is inferred to be the consequence of the enhanced amplitudes of oxygen atoms in the phonon mode. Finally, spin-phonon coupling parameters are computed in a Heisenberg formulism. They reveal the changes in exchange couplings due to specific atomic displacements or phonon modes, as well as the inequality of the out-of-plane exchange couplings across LaO layers and across SrO layers, the latter being the result of the artificial structuring in the superlattice.

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