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Density functional study of ferromagnetic ferroelectric $LaMnO_3/BaTiO_3$ superlattice[1] LEONARD KLEINMAN, BHAGAWAN SAHU, ADRIAN CIUCIVARA, University of Texas at Austin — Using the GGA + U density functional, we have calculated the lattice constants, atomic positions, magnetization, and ferroelectric polarization of a $(LaMnO_3)_{4.5}(BaTiO_3)_{4.5}$ superlattice containing five LaO and TiO_2 planes and four MnO_2 and BaO planes. Although $LaMnO_3$ is antiferromagnetic, it is ferromagnetic in the superlattice. An approximation to the ferroelectric polarization, obtained from a comparison of superlattice and bulk crystal atomic displacements and unit cell volumes, is found to agree reasonably well with the polarization obtained from a Berry phase calculation. The electric polarization points along the longer in-plane lattice vector, while the atomic spins, after the spin-orbit interaction and spin noncollinearity are included, all point in directions close to that lattice vector.

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