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Ab Initio Studies of Magnetoelectric Coupling at $PbZr_{0.2}Ti_{0.8}O_3/La_{0.8}Sr_{0.2}MnO_3$ and $PbZr_{0.2}Ti_{0.8}O_3/La_{0.5}Sr_{0.5}MnO_3$ Multiferroic Interfaces KRISHNA ACHARYA, IGOR VASILIEV, Department of Physics, New Mexico State University, Las Cruces, NM 88003 USA — The magnetic properties of multiferroic materials can be controlled by the applied electric field. In this work, we use *ab initio* methods based on density functional theory (DFT) to study the magnetoelectric coupling at the (0,0,1) interface between PZT ($PbZr_{0.2}Ti_{0.8}O_3$) and LSMO at two different doping levels ($La_{0.8}Sr_{0.2}MnO_3$ and $La_{0.5}Sr_{0.5}MnO_3$). A $\pm 1\%$ uniaxial strain is applied to modeled system in the direction orthogonal to the LSMO/PZT interface. We observe a transition from the ferromagnetic (FM) to antiferromagnetic (AFM) state at the $PbZr_{0.2}Ti_{0.8}O_3/La_{0.5}Sr_{0.5}MnO_3$ interface under the applied strain. In contrast, no FM/AFM transition is observed at the $PbZr_{0.2}Ti_{0.8}O_3/La_{0.8}Sr_{0.2}MnO_3$ interface. The results of our calculations are consistent with the available experimental data.

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