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First-Principle Study of the $La_{0.67}Sr_{0.33}MnO_3/PbZr_{0.2}Ti_{0.8}O_3$(001) Interface[1] MAHMOUD HAMMOURI, New Mexico State University, EDWIN FOHTUNG, New Mexico State University and Los Alamos National Laboratory, ROSS HARDER, Argonne National Laboratory, VALERIA LAUTER, Oak Ridge National Laboratory, IGOR VASILIEV, New Mexico State University — Multiferroic heterostructures composed of thin layers of ferromagnetic and ferroelectric perovskites have attracted considerable attention in recent years. We apply *ab initio* computational methods based on density functional theory to study the characteristics of the magnetoelectric coupling at the (001) interface between $La_{0.67}Sr_{0.33}MnO_3$ (LSMO) and $PbZr_{0.2}Ti_{0.8}O_3$(PZT). The calculations are carried out using the Quantum ESPRESSO electronic structure code combined with Vanderbilt ultrasoft pseudopotentials. Our study shows that the interfacial interaction between LSMO and PZT and the polarization of PZT have a strong influence on the distribution of magnetization within the LSMO layer. A significant change in the magnetization of the LSMO layer adjacent to PZT is observed after reversal of the direction of polarization of PZT.

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