

Abstract: NeSA202100poster-10: *Ab Initio* Study of the Effects of Strain and Doping on the Properties of LSMO/PZT Multiferroic Interfaces

Time: 12:00-1:00 PM

Presenter:

Krishna Acharya

Authors:

¹Krishna Acharya, ¹Igor Vasiliev

¹*Department of Physics, New Mexico State University, Las Cruces, New Mexico 88003, USA*

We apply *ab initio* methods based on density functional theory (DFT) to study the influence of strain and doping on the magnetoelectric coupling at the (0,0,1) interface between PZT $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ and LSMO at three different doping levels $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$, $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ and $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$. The effects of strain are modeled by applying a 1.5%, uniaxial strain in the direction orthogonal to the LSMO/PZT interface. Our calculations show that the magnetic properties of the LSMO layer are strongly influenced by both the doping concentration and the applied uniaxial strain. The results of our study are consistent with the available experimental data.