World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:8, No:05, 2014

Half-Metallicity in a BiFeO3/La2/3Sr1/3MnO3 Superlattice: A First-Principles Study

Authors : Jiwuer Jilili, Ulrich Eckern, Udo Schwingenschlogl

Abstract : We present first principles results for the electronic, magnetic, and optical properties of the BiFeO3 /La2/3Sr1/3MnO3 heterostructure as obtained by spin polarized calculations using density functional theory. The electronic states of the heterostructure are compared to those of the bulk compounds. Structural relaxation turns out to have only a minor impact on the chemical bonding, even though the oxygen octahedra in La2/3Sr1/3MnO3 develop some distortions due to the interface strain. While a small charge transfer affects the heterointerfaces, our results demonstrate that the half-metallic character of La2/3Sr1/3MnO3 is fully maintained.

Keywords : BiFeO3, La2/3Sr1/3MnO3, superlattice, half-metallicity
Conference Title : ICMSCMP 2014 : International Conference on Material Science and Condensed Matter Physics
Conference Location : Berlin, Germany
Conference Dates : May 22-23, 2014