

## Half-Metallicity in a BiFeO<sub>3</sub>/La<sub>2</sub>/3Sr<sub>1</sub>/3MnO<sub>3</sub> 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 BiFeO<sub>3</sub>/La<sub>2</sub>/3Sr<sub>1</sub>/3MnO<sub>3</sub> 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 La<sub>2</sub>/3Sr<sub>1</sub>/3MnO<sub>3</sub> 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 La<sub>2</sub>/3Sr<sub>1</sub>/3MnO<sub>3</sub> is fully maintained.

**Keywords :** BiFeO<sub>3</sub>, La<sub>2</sub>/3Sr<sub>1</sub>/3MnO<sub>3</sub>, 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