

Abstract Submitted
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First-principles study of magnetic, electronic and optical properties of double perovskite $\text{Bi}_2\text{FeMnO}_6$ ¹ TOWFIQ AHMED, DZMITRY YAROTSKI, QUANXI JIA, JIAN-XIN ZHU, Los Alamos Natl Lab — We study magnetic, electronic and optical properties of double perovskite $\text{Bi}_2\text{FeMnO}_6$ (BFMO) using density functional theory. In these systems, the exchange interaction between Fe and Mn sites gives rise to a ferrimagnetic ordering, which is captured in our ab initio calculations. Thin film $\text{Bi}_2\text{FeMnO}_6$ (BFMO) are generally grown on substrates such as SrTiO_3 and Si. Significant strain has been experimentally observed in BFMO unit cells due to slight lattice mismatch between the thin film and substrate unit cells. In this work, we find that the net magnetic moment in BFMO depends on the “c/a” ratio of the unit cell, suggesting the strain dependence of magnetization in such system. We further calculate x-ray magnetic dichroism (XMCD) signals of Fe and Mn ions in BFMO for L2 and L3 edges. By applying the XMCD sum rules, we adopted an alternative approach to estimate the spin and orbital magnetic moment from our DFT calculations. We find qualitative agreement between our calculated values and the experimental measurements based on different techniques. Moreover, we study spin resolved optical conductivity and density of states in BFMO. These calculations give insight into electronic structure near Fermi energy, and dominant electronic excitations in the valence-conduction region of BFMO.

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