Structural and electronic properties of Ba_2TiMnO_6 studied by DFT calculations

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Magnetically ordered perovskite-like materials show semiconductor properties with their promised applications in the optoelectronic industry. In this work, we report *ab-initio* calculations of electronic structure and magnetic properties of the Ba_2TiMnO_6 double perovskite. Calculations are carried out through the Full-Potential Linear Augmented Plane-Wave method (FP-LAPW) within the framework of the Density Functional Theory (DFT) using several common approximations: Local Density (LDA) [1] and Generalized Gradient (GGA) approximations [2] by including the relativistic effects of spin-orbit coupling with the Hubbard term corrections GGA+U. However, a good agreement is obtained for Ba_2TiMnO_6 with the previously reported data by Deluque Toro *et al.* [3], there are essential differences in the case of GGA and GGA+U approaches due to reliable lattice parameters after optimization. The study of the electronic structure was based in the analysis of the density of state (DOS), and the electronic band structure (EBS), indicating that this compound evidences an effective magnetic moment of 2.56 μ_B/Mn and the distinct energy gap of about 1.23 eV. On the other hand, the magnetic moment of Mn decreases in case of the effect of the Hubbard parameter U (U=4 eV, J=1 eV) and obtains 2.28 μ_B per Mn ion and the band gap is wider achieving 1.54 eV. The obtained results indicate that Ba_2TiMnO_6 is a direct band gap semiconductor.

References:

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