Abstract

Double perovskite compounds are among the most researched materials due to their intriguing
physical and chemical characteristics, as well as the variety of applications resulting from their structures' adaptable composition. Despite a great deal of effort, the magnetic structure of Ba_2MnWO_6 (BMW) and certain distortions in the crystal structure of Ba_2TiMnO_6 (BTM) remain inconsistent with theoretical and empirical conclusions. By thoroughly establishing the magnetic phase stability and elucidating the electronic structure and optical properties of these double perovskites, we hope to uncover additional details regarding the mechanisms behind their semiconducting activity. Utilizing the advanced capabilities of DFT theory, we investigated electronic structure properties (Density of States (DOS), Electronic Band Structure (EBS), and Electron Localization Function (ELF)), and optical properties (dielectric function, refractive index, extinction coefficient, reflectivity, energy-loss function, absorption spectrum, and optical conductivity) employing the Full Potential Linearized Augmented Plane Wave (FP-LAPW) and Pseudo-Potential Projector Augmented Wave (PP-PAW) methods.

With collinear Mn spins oriented the [001] direction and an ordered moment μ_{ord} of approximately 4.42 μ_B for BMW and 2.56 μ_B for BTM, our results indicate that the most stable magnetic structure is antiferromagnetic. Following the thorough examination of the electronic band structure (EBS) and density of states (DOS), it can be determined that BMW is an indirect narrow band gap semiconductor with a semiconducting energy gap of roughly E_g = 0.36 eV, while BTM is a direct band gap semiconductor with a gap E_g of 0.98 eV.

Furthermore, the impact of Hubbard correction terms U_{eff} on the semiconducting energy gap E_g was investigated. Unlike μ_{ord}, E_g increases with U_{eff}, reaching 1.76 eV for BMW and 1.27 eV for BTM at U_{eff} = 3 eV. These findings also suggest that transition metal atoms play a crucial role in defining the lattice constants in double perovskite compounds. In addition, the distinction between spin-up and spin-down states in DOS structures shows the magnetic order of Mn^{2+} moments. The magnetic order in BTM is created by the super-exchange interaction, which involves electron hopping between the Mn-3d and O-2p orbitals. Both double perovskites have high optic conductivity, dielectric constants, and a strong ultraviolet light absorption coefficient, making them excellent candidates for high-performance perovskite
solar cells in optoelectronic applications. Using the Projected Augmented Wave (PAW) approach, we studied how pressure affects the crystal structure and DOS of Ba_2TiMnO_6. Our findings indicate that under compressive strain at pressures of 8 GPa,