

# Ab initio study of structural, electronic and optical properties of the perovskite CeFeO<sub>3</sub> compound

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**Abstract:** In recent years perovskite materials have attracted great attention in the field of photovoltaic energy. A theoretical study of these compounds proves great importance to help researchers in their experimental choice. The full-potential linearized augmented plane wave (FP-LAPW) method in the framework of density functional theory (DFT) implanted in the Wien2k code is applied to the study of structural, electronic and optical properties of CeFeO<sub>3</sub>. We have used the generalized Perdew Burke Ernzerhof gradient approximation (PBE-GGA) as well as the Becke-Johnson modified exchange potential (TB-mBJ) to correct the gap's energy. The gap energy results of 1.19 eV obtained using mBJ are reasonable compared to the available experimental data (1.77eV). The asymmetry in the total density of state (DOS) deduced from band structure calculation confirms the marked magnetic character of CeFeO<sub>3</sub>. Our results highlight that it is possible to obtain a magnetic semiconductor with an interesting gap band ( $\approx 1.2$  eV), which is promising for applications in photovoltaics.

*Keywords:* Perovskite, Functional Density Theory (DFT), TB-mBJ, PBE-GGA, Photovoltaic application.

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