Ab initio insights into the physical properties of cubic $CeFeO_3$ perovskite

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Abstract

We used the full-potential linearized augmented plane wave (FP-LAPW) method to study different features of the structural, mechanical, optoelectronic and charge transport behavior, of cubic perovskite $CeFeO_3$. To handle the exchange and correlation potential, we applied two different methods: GGA-PBE and mBJ-GGA. The ferromagnetic (FM) state of $CeFeO_3$ is confirmed to be more stable by comparing total energy variations with changes in unit cell size. To address the exchange and correlation potential, we employed two different approximations: GGA-PBE and mBJ-GGA. The structural and thermodynamic stability was confirmed by the formation energy, cohesive energy and tolerance factor. Analysis of the energy band structure using the GGA-PBE method within the generalized gradient approximation framework confirms the material's metallic properties. Additionally, the enhanced band gap of 2.87 eV has been found for $CeFeO_3$ is calculated using the TB-mBJ approach spin-down channel. According to optical outcomes, the wide range of absorption in the ultraviolet region indicates the potential candidates for optoelectronic applications. Based on

magnetic properties, $CeFeO_3$ has a magnetic moment (μB) of 6.000 μB. The integral values of the magnetic moment determine the nature of ferromagnetism (FM). The Boltzmann transport analysis conducted using the BoltzTraP tool examined the thermoelectric characteristics. The compound $CeFeO_3$ showed a figure of merit (ZT) value close to one at room temperature, suggesting it could be used to create very efficient thermoelectric devices. © 2026 Elsevier B.V.

Author keywords

Absorption coefficient; DFT; Halfmetallicity; Seebeck coefficient

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