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Ab initio insights into the physical properties of cubic CeFeO3 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 CeFeO₃. To handle the exchange and correlation potential, we applied two different methods: GGA-PBE and mBJ-GGA. The ferromagnetic (FM) state of CeFeO₃ 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 CeFeO₃ 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, CeFeO₃ has a magnetic moment (μ_B) of 6.000 μ_B. 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 CeFeO₃ showed a figure of merit (ZT) value close to one at room temperature, suggesting it could be used to create very efficient thermoelectric devices.
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Data availability statement

The data can available on the reasonable request to the corresponding authors. 9 A. Nazir et al. Computational Condensed Matter 47 (2026) e01312

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