

Área: FIS

The influence of magnetism on the chemical bond of CaFeO₃ material

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Highlights

Superexchange interactions depend on the mechanisms of spin polarization and localization.

The spin localization on the O atoms is fundamental to explain the magnetic ordering of the CaFeO₃ material.

Abstract

Superexchange model described by Goodenough-Kanamori-Anderson is essential physical model for magnetism and material science. The interaction between unpaired electrons mediated by p orbitals of non-magnetic atoms in a structure describes the magnetic ground state. But the GKA model is limited in distorted material and lacks and is not representative of materials with distortions or defects such as structural doping, substitutions, vacancies and surfaces. In CaFeO₃ perovskite material in cubic and orthorhombic phases is reported to exhibit experimental and theoretical discordances in predicting the magnetic ordering of the material. In present works, simulations with DFT/B3LYP calculation level, CaFeO₃ material in cubic and orthorhombic symmetry exhibits FM and A-AFM magnetic ordering respectively. Magnetic ordering is dependent on geometry because it is a direct influence of electronic structure in different lattice arrangements. Variation of magnetic orderings exhibits modulations in chemical bond profile, which FM exchange induces antibonding states while AFM induces bonding. Each polymorph and magnetic ordering exhibit a specific spin polarization and localization that effectively couples unpaired electrons. The spin localization mechanism is fundamental to understanding the role of O in superexchange in CaFeO₃ material. The localization mechanism separated α and β electrons to coupling magnetic cations of structure.

References

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