

Computational Determination of the Magneto-electronic Properties of $Ce_{1-x}Cu_xO_2$ ($x=12.5\%$): Emerging Materials for Spintronic Devices

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Introduction

Ceria (CeO_2) is used in a wide range of applications, it has many interesting physical properties like its high oxygen storage capability; consequently, this material has a wide range of applications covering catalytic industry, superconductivity and solid oxide fuel cells [1,2]. It is a promising component in catalytic converters to reduce harmful emissions from automobile exhausts [3]. In the present work, we investigated the structural, electronic and magnetic properties of copper-doped CeO_2 . The Cu transition metal is used as a dopant agent to persuade spin polarization in CeO_2 compound.

Simulation Methodology

Doping CeO_2 with transition metals is an effective way of tuning its properties. In the present work we have performed self-consistent ab-initio calculation using the full-potential linearized augmented plane-wave method (FP-LAPW), based on the density functional theory (DFT) as implemented in the Wien2k simulation code [4] to study the structural, electronic and magnetic properties of the compound $Ce_{1-x}Cu_xO_2$ ($x=12.5\%$) fluorite type oxide and to explore the effects of dopant Cu in ceria. The exchange correlation potential has been treated using the Perdew-Burke-Eenzerhof revised of solid (PBEsol).

Results and Discussion

In structural properties, the equilibrium lattice constant is observed for the compound, which exist within the value of 5.382 \AA . To calculate the electronic nature of this compound, the band configuration of $Ce_{1-x}Cu_xO_2$ ($x=12.5\%$) for both spin-up and spin-down configuration are simulated, and elucidates the semiconductor nature of material. It has indirect band gap for both spin channels as represented in figure 1 with the compound was observed to have a narrow band gap on the spin-down configuration (0.162 eV) and band gap on the spin-up (2.067 eV). Hence, the doped atom Cu play a vital role in increasing the magnetic moments of the super cell and the value of the total magnetic moment is found to be $2.99438 \mu_B$.



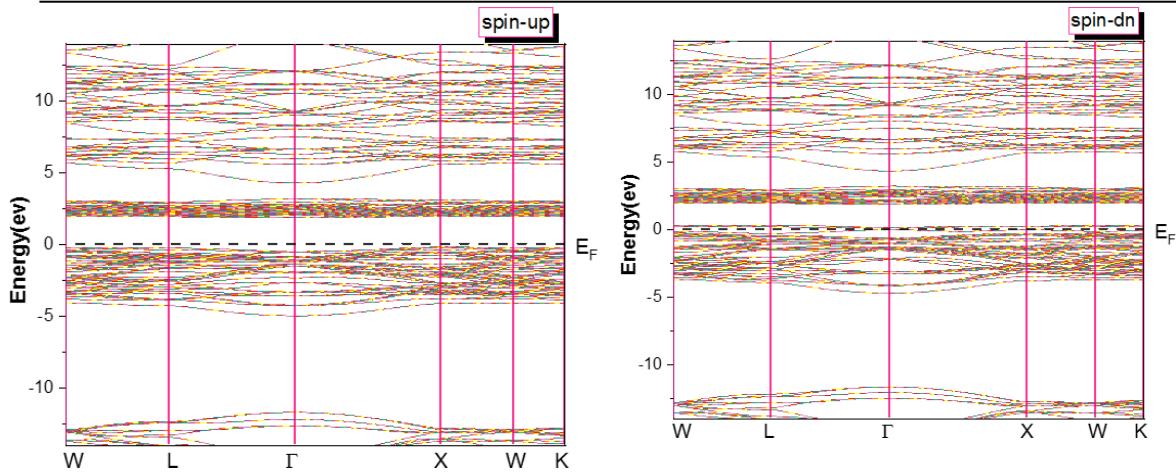


Fig. 1. Spin-polarized energy band plots of Cu-doped CeO₂.

Conclusion

Structural, electronic and magnetic properties of Ce_{1-x}Cu_xO₂ (x=12.5%) examined by using the Wien2K code via DFT computations. Cu doping in CeO₂ has confirmed the semiconductor ferromagnetism. The predicted results propose the compound could be a good candidate for spintronic applications.

References

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