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

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Abstract : 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 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). In structural properties, the equilibrium lattice constant is observed for the compound, which exists within the value of 5.382 A°. In electronic properties, the spin-polarized electronic bandstructure elucidates the semiconductor nature of the material in both spin channels, with the compound was observed to have a narrow bandgap on the spin-down configuration (0.162 EV) and bandgap on the spin-up (2.067 EV). Hence, the doped atom Cu plays a vital role in increasing the magnetic moments of the supercell, and the value of the total magnetic moment is found to be 2.99438 μB. Therefore, the compound Cu-doped CeO_2 shows a strong ferromagnetic behavior. The predicted results propose the compound could be a good candidate for spintronics applications.

Keywords : Cu-doped CeO_2, DFT, Wien2k, properties
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