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Electronic structure and band profile in cubic $CeCoO_3$: A rare earth perovskite

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Since the discovery of perovskites, they have become true engineering ceramic material with a plethora of novel applications covering almost all the frontier areas of modern technology, like, fuel cell technology, radioactive waste encapsulation, dielectric resonator materials, etc. Strong interaction occurring in spin and charge states of the perovskites makes them a promising candidate for multiferroic (with both magnetic and ferroelectric ordering) materials. The giant magneto-resistance effect brought a revolution in the field of spintronics or magneto-electronics leading to the significant promotion of magnetic memory technology.

Rare-earth (RE) cobaltates with a general structural formula $ACoO_3$ have been a subject of interest from the past few decades due to their unique characteristics like superconductivity, colossal magneto-resistance, sensing effects, low temperature magnetic behavior, catalytic activity, and electronic structure complexion. Mainly focused among such materials are of the kind $RCeCoO_3$ (where R = La, Ce, Pr, Nd, Sm). Being, the promising and efficient candidates for optoelectronic, spin-state and memory devices, the physical properties of these materials are highly desirable.

Present study has been carried out to investigate the electronic and magnetic behavior of cubic $CeCoO_3$ perovskite. The first principle calculations with highly precise spin-polarized density functional theory have been performed to study the electronic and magnetic properties of $CeCoO_3$ cubic perovskite. The perovskite $CeCoO_3$, crystallizes in cubic Pm-3m structure, where atoms are located as Ce (0,0,0), Co (0.5,0.5,0.5) and O (0,0.5,0.5), (0.5,0,0.5) (0.5,0.5,0) sites. The six O atoms surround a Co atom at the body-centre position. The supercell optimizations for this material in all the three phases (I.e. NM, FM and AFM) expose its ground state to be the antiferromagnetic one, which yield the optimized lattice constant a = 3.79 Å with bulks modulus (B) = 192.3 GPa.

In order to elucidate the formation of band structure, the total density of states (DOS) for both the spin states of $CeCoO_3$ are presented in Figure 1. From the band structure, total and partial density of states, the half metallic behavior with an indirect band gap of 2.7 eV between the conduction minima and valence maxima, is seen in the high spin phase. Total and partial densities of states robustly reveal the Co atom to be the main contributor towards the magnetism in this compound.

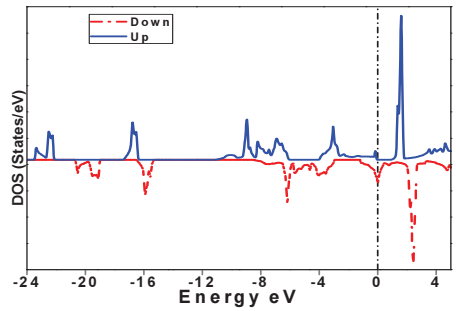

Figure 1: Spin-polarized total density of states (DOS) at equilibrium lattice constant for $CeCoO_3$. The Fermi level is set at zero energy

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