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Band Profile Comparison of the Cubic Perovskites $CaCoO_3$ and $SrCoO_3$

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Structural geometries, electronic band structures, spin densities, and magnetic properties of the cubic perovskites $CaCoO_3$ and $SrCoO_3$ are studied using the highly accurate spin-polarized density functional theory. It is found that the structural parameters and geometry of $SrCoO_3$ are consistent with experimental results. Careful analysis of the band profiles reveals that the overall electronic band structure of $CaCoO_3$ is similar to the electronic band structure of $SrCoO_3$, with a small difference in details. The total and partial densities of states show that $CaCoO_3$ and $SrCoO_3$ compounds are ferromagnetic metals. The calculated magnetic moments of these compounds also reveal that they are ferromagnets. Furthermore, the comparison of the calculated magnetic moments for Co and $SrCoO_3$ is consistent with experimental results, confirming the validity of our theoretical results. On the basis of the presented electronic structure and magnetic properties, it is expected that $CaCoO_3$ is also a colossal magnetoresistive material like $SrCoO_3$.

Key words: CMR, ferromagnetic metals, magnetic perovskites, crystal field splitting

INTRODUCTION

Cobalt-based oxides are attractive materials for applications in solid-state fuel cells and gas separation membranes.[1] Interest in these compounds has grown in recent years after the discovery of superconductivity and colossal magnetoresistivity in some Co-based compounds.[2] The rich physical properties of Co-based compounds can be related to the closeness of the crystal field splitting (E_{CF}) and the exchange energy (E_{ex}) (Hund's coupling rule) of Co^{3+} in the octahedral coordination, with a small energy difference between the low-spin (LS) state t_{2g} 6 e_g 0 ($S = 0$), the intermediate-spin (IS) state t_{2g} 5 e_g 1 ($S = 1$), and the high-spin (HS) state t_{2g} 4 e_g 2 ($S = 2$).[3] New theoretical and experimental techniques are used to investigate the coupling between magnetic and orbital degrees of freedom, which play a major role in the study of these materials.[2] Most of the interesting physical properties in transition-metal oxides are due to the interdependence of the structural, electronic, magnetic, and optical properties. These compounds are expected to be efficient materials for spin-based electronics (spintronics).

The physical properties of perovskites are highly desirable because they reveal many fascinating properties such as high thermoelectric power, superconductivity at high temperature, ferroelectricity, charge ordering, colossal magnetoresistance (CMR), and spin-dependent transport.[4] These materials have frequently attracted enormous attention for applications as sensors, substrates, and catalytic electrodes, and are also promising candidates for advanced microelectronic, optoelectronic, and spintronic devices.[5]

$SrCoO_3$ possesses an extremely symmetric cubic structure.[1] The reported lattice constant of the cubic perovskite $SrCoO_3$ is 3.892 Å,[6] while the Co–O bond length is 1.912 Å.[3] $SrCoO_3$ samples are prepared from SrO_2 and Co_3O_4 raw materials under ambient and high pressure.[6] $SrCoO_3$ contains both Co^{3+} and Co^{4+} ions, while magnetic measurements show the metallic ferromagnetic nature of the compound,

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