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Electronic structure and magnetic ground state properties of $SrCoO_{2.5}$[1] CHANDRIMA MITRA, RANDY S. FISHMAN, SATOSHI OKAMOTO, HO NYUNG LEE, FERNANDO A. REBOREDO, Oak Ridge National Laboratory — $ABO_{3-\delta}$ type perovskite oxides are potential candidates for solid oxide fuel cells. The ones that crystallize in the orthorhombic brownmillerite-phase ($ABO_{2.5}$), such as $SrCoO_{2.5}$, are particularly interesting due to their crystal structure which contains ordered channels of oxygen vacancies. In this work we investigate theoretically the ground state electronic structure and magnetic properties of the brownmillerite phase of $SrCoO_{2.5}$. Strong correlations of the Co d electrons are treated within the local spin density approximations of Density Functional theory (DFT) with Hubbard U corrections (LSDA+U). The results are compared with the Heyd Scuzeria Ernzerhof (HSE) functional. The parameters computed with a U value of 7.5 eV are found to match closely to those computed within the HSE functional. Consistent with experimental observation a G-type antiferromagnetic structure is found to be the most stable one. From a Heisenberg Hamiltonian we compute the magnetic exchange interaction parameters, J, between the Co atoms which are then used to compute the spin-wave frequencies and inelastic neutron scattering intensities. The system has four spin-wave branches. The lowest energy mode was found to have the largest scattering intensity at the magnetic zone center.

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