

Origin of Metal–Insulator Transition in n -doped ABO₃ Perovskite Metals

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A subclass of ABO₃ perovskite (PV) metals is known to undergo metal-to-insulator transitions (MITs) when n -doped. Particularly, the PV ferromagnet, strontium cobaltite (SrCoO₃), undergoes an MIT when a critical level of ordered oxygen vacancies are present in the system. Concomitant topotactic and magnetic transitions can also occur, e.g., the oxygen-deficient SrCoO_{2.5} phase is an anti-ferromagnet and the vacancies order forming a brownmillerite crystal structure. The cause of this nonintuitive MIT in these oxygen-deficient systems, where strong correlation is present, has not been precisely described, however, density functional calculations suggest charge disproportionation is often associated with the transition. Also, counting of formal oxidation states in the oxygen-rich systems hints at the presence of ligand holes which would conceivably lead to passivization after n -doping. Here, we hypothesize that these systems are indeed self-hole doped and use the explicitly correlated diffusion Monte Carlo method to gain clarity on the electronic/magnetic/structural transitions.