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Density functional modeling for a perovskite $SrTi_{1-x}Co_xO_3$ system: Beyond GGA+U functional¹ JUAN MANUEL FLOREZ, Massachusetts Institute of Technology and Universidad Técnica Federico Santa María, SHYUE PING ONG, GER-BRAND CEDER, GERALD F. DIONNE, Massachusetts Institute of Technology, PATRICIO VARGAS, Universidad Técnica Federico Santa María, CAROLINE A. ROSS, Massachusetts Institute of Technology — Understanding the exact mechanisms of spin-stabilization according to the oxygen stoichiometry and substituting metal-transition ions is essential to finding new perovskites-based technologies to augment silicon-based devices with room-temperature spintronic materials. We perform ab-initio modeling for the $\text{SrTi}_{1-x}\text{Co}_x\text{O}_3$ system with x = 0.0, 0.25, 1.0, and by using a HSE06 hybrid functional. Electronic structure for x=(0.0,1.0) predicts 3.1 eV band gap and a metallic behavior, respectively, predicting lattice parameters in agreement with experiments. Different positions for the cobalt ions are taken into account for x=0.25, and predicted ground states and Co energy-correlations suggest the structurally stabilized Co-site positions as fingerprints of whether possible intrinsic magnetic ordering or other phenomena is giving rise to the macroscopic magnetism. Passing from Stoichiometric SrTi_{0.75}Co_{0.25}O₃ to 1-O-vacancy $SrTi_{0.75}Co_{0.25}O_{3-\delta}$ produces a lattice parameter expansion due to the valence state distribution of the substituting B (ABO_3) ions, which is turn lead us to a band gap expansion. The stabilized valence spin states of the magnetic ions are discussed in comparison with Juan Manuel Florez the ligand-field theory. Massachusetts Institute of Technology and

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