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Looking for multiferroics through oxygen deficiency in $\mathbf{SrTi_{1-x}(Fe_x,Co_x)O_{3-\delta}}$ JUAN MANUEL FLOREZ, Technical University Federico Santa Maria (Chile) and MIT, MEHMET CENGIZ ONBASLI, DONG HUN KIM, MIT (USA), SHYUE PING ONG, University of California at San Diego, GERBRAND CEDER, MIT (USA), PATRICIO VARGAS, Technical University Federico Santa Maria (Chile), CAROLINE A. ROSS, MIT (USA) — We present a theoretical/experimental study of $AB_{1-x}B'_xO_{3-\delta}$ magnetic perovskites obtained by solid solution of Fe and Co into $SrTiO_3$. We focus on the role of the oxygen deficiency as the factor triggering both a change of the saturation magnetization and the apparition of a macroscopic electric polarization. The magnetism is analyzed by calculating the $t_{2g}e_g$ occupancies of the magnetic cations for different O-deficiencies (δ), substitution values (x) and FM/AFM orderings as well as the electric polarization is studied through the non-centrosymmetric resulting structures generated by the intrinsic strain related to the oxygen holes and changes of the ions radii. The optical properties are quantified by calculating the total and projected density of states while we take into account all the possible configurations of the O-vacancies respect to different B′ locations at the supercells. Ab-initio results are compared with experimental on es for $SiTr(Fe,Co)O_3$ and we show that a stable multiferroic state seems to be possible for intermediate values of the oxidation and magnetic composition as suggested by the agreement between modeling and experiments.

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