

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**An oxygen-deficiency modulated multiferroic: Cobalt-substituted perovskite**<sup>1</sup> JUAN MANUEL FLOREZ, Universidad Tcnica Federico Santa Mara; Massachusetts Inst. of Tech. — In this work, we use density functional theory to model recently demonstrated room temperature ferromagnetism and ferroelectricity in polycrystalline and single crystal Cobalt-substituted SrTiO<sub>3</sub> thin films (SrTi<sub>0.70</sub>Co<sub>0.30</sub>O<sub>3-d</sub>), deposited at different oxygen pressures to change their oxygen vacancy concentration. The modeling indicates an origin for both magnetism and electric polarization in the interactions between oxygen vacancies and the B-site cations. The magnetization saturation increases with the oxygen deficiency as a result of valence spin states changes, which depend on whether the oxygen octahedral of the respective local B-site cations are complete or not. On the other hand, a finite electric polarization appears as a result of a non-centrosymmetric distribution of different resulting local charges and such a polarization increases when the oxygen vacancies increase. Increasing of both order parameters, magnetic and ferroelectric, are analyzed respect to all possible Co-sites and O-vacancies distributions, showing that these results suggest a class of multiferroic materials with properties controlled by their oxygen stoichiometry. Agreement and discrepancies between experiments and modeling are discussed.

<sup>1</sup>J M Florez and P Vargas thank Fondecyt 1130950 and 11130128, all authors thank the MISTI MIT-Chile, and CAR thanks the (S3TEC) and DoE under DE-SC0001299

Juan Manuel Florez  
Universidad Tcnica Federico Santa Mara; Massachusetts Inst. of Tech.

Date submitted: 25 Nov 2015

Electronic form version 1.4