Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Crystal structure and electronic properties of bulk and thin-film brownmillerite oxides JOSHUA YOUNG, Drexel University, JAMES RONDINELLI, Northwestern University — The equilibrium structure and functional properties exhibited by brownmillerite oxides (general formula $A_2B_2O_5$), a family of perovskite-derived structures with alternating layers of BO_6 octahedra and BO_4 tetrahedra arising from ordered arrangements of oxygen vacancies, is dependent on a variety of competing crystal-chemistry factors. Using first principles electronic structure calculations, we investigate two antiferromagnetic brownmillerite ferrites, $Sr_2Fe_2O_5$ and $Ca_2Fe_2O_5$, and find that the stability of the equilibrium ground state is governed by complex interactions among several structural descriptors, including ionic size, distortions of nominally regular oxygen octahedral, and in-plane and out-of-plane separation of tetrahedral chains. Furthermore, we find that these same effects control the preferred oxygen vacancy orientation under epitaxial strain, a tunable parameter which also strongly influences the magnitude of the electronic band gap via an asymmetric-vacancy alignment dependent response. Finally, we show that A-site cation ordering in these materials can lift inversion symmetry, providing a potential new route to room temperature multiferroics.

Joshua Young
Drexel University

Date submitted: 06 Nov 2015 Electronic form version 1.4