Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Directing and harnessing anion order in YBaFe2O5F oxyfluoride perovskites STEVEN HARTMAN, ARASHDEEP THIND, ROHAN MISHRA, Washington Univ — article Anion ordering in mixed-anion transition metal perovskites, such as oxyfluorides, offers a new route to control their properties and achieve novel functionalities. However, O/F ordering is limited by entropy in oxyfluorides synthesized through traditional solid-state techniques, which require high temperatures. Here, using total energies and activation barriers from first-principles density functional theory calculations, we show that it is possible to achieve O/F order using topochemical fluorination of oxide perovskites having ordered oxygen vacancies. We use $YBaFe_2O_5$ as a representative compound, which has oxygen vacancies that are ordered in the Y-layers. We find that fluorination is most favorable at the oxygen vacancy site in the Y-layers, which leads to polar building units with finite dipole moment due to alternating layers of BaO and YF about the FeO_2 layers. We will discuss these findings along with the predicted electronic and magnetic properties of $YBaFe_2O_5$ with O/F order.

Steven Hartman
Washington Univ

Date submitted: 11 Nov 2016 Electronic form version 1.4