Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Strain control of magnetic structure in layered iridates via strong orbital-lattice coupling CHOONG HYUN KIM, CRAIG FENNIE, Cornell Univ
— We have studied from first principles the structural, electronic, and magnetic properties of the layered-perovskite iridates A_2IrO_4 and $A_3Ir_2O_7$ (A=Sr,Ba) as a function of epitaxial strain. In most of perovskite iridates, due to their large spin-orbit coupling and cubic crystal field, ground state could be described by an effective total angular momentum state $J_{\text{eff}} = 1/2$ within t_{2g} manifold. In contrary to what is usually assumed, we find that $d_{x^2-y^2}$ orbital plays a crucial role to determine a magnetic ground state of iridates if the cubic crystal field is not big enough compared to band width. For instance Ba_2IrO_4 with tensile strain induces a situation in which magnetization is reversed. Our first-principles results show how A-site cation, dimensionallity, and strain are correlated with the band width and crystal field to control magnetic ground states.

Choong Hyun Kim
Cornell Univ

Date submitted: 14 Nov 2014 Electronic form version 1.4