Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Hund's coupling and spin-orbit coupling in iridates revisited** HUA CHEN, GURU KHALSA, ALLAN H. MACDONALD, University of Texas at Austin — In recent years iridates have attracted a lot of interests because of unusual properties due to a combination of strong correlations and strong spin-orbit scattering. The magnetic properties of these materials are often analyzed theoretically by applying the Kugel-Khomskii model and specifically considering the $J = \frac{1}{2}$ subspace decoupled by strong spin-orbit coupling. It is not obvious that such an approach is always valid, however, given that the spin-orbit coupling, on-site correlation energies, intra-atom exchange energies, tetragonal splittings, etc. all have comparable strength. In this work we will revisit the magnetic interactions of these materials combining insights from an examination of the 2-electron multiplet structure of a $t_{2g}$ ion using the Slater theory of atomic structure, and ab initio electronic structure calculations. We will also discuss the the magnetic anisotropy and domain-wall energies of specific iridate materials implied by these magnetic interactions.

Xiao Li
Department of Physics, The University of Texas at Austin

Date submitted: 29 Nov 2012 Electronic form version 1.4