Condensed Matter / Biophysics Seminar

Thursday

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4:00 P.M.

Rm 184 NSH

X-ray spectroscopy and high-pressure tuning of the spin-orbit coupled ground state of Iridate oxides

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Electrons in atoms have both spin and orbital motions. The coupling of these motions (S-O coupling) is responsible for fine structure in the absorption/emission spectra of atoms and the inclusion of spin-orbit interactions is necessary for a correct description of atomic structure. This weak (relativistic) interaction, however, is rarely important in understanding the behavior of solids. This is because the properties of solids are determined by outer, valence electrons subjected to crystal electric fields, band formation and Coulomb electron-electron interactions usually much stronger than S-O coupling. This is certainly the case in first-row (3d) transition metal oxides such as Cu- and Fe-based high Tc superconductors, and Mn-based colossal magneto resistive manganites and multiferroics.

Recently, third-row transition metal oxides based on Iridium atoms with half-filled 5d shells ($5d^5$, Ir4+ ions) have generated great interest due to the observation of unconventional insulating and magnetic ground states [1]. Since the spatial extent of $5d$ wave functions is significantly larger than their $3d$ analogs, strong band effects would usually lead to itinerant-like behavior and absence of local moments due to concomitant decrease in Coulomb interactions. Strong S-O interactions in heavy Ir ions, however, appear to be responsible for the novel behavior.

We used x-ray resonant absorption and scattering techniques to probe the nature of the electronic ground state in magnetic insulators $BaIrO_3$ and Sr_2IrO_4 [2, 3]. A spin-only description of the magnetic ground state is directly ruled out by the measurements. Instead, the measurements show spin-orbit entanglement in $5d$ states resulting in comparable orbital (L_z) and spin (S_z) contributions to the local magnetic moment, even in the presence of strong crystal field and band effects. Experiments at high-pressures [3] present a unique opportunity for tuning the delicate interplay between electronic bandwidth, S-O and Coulomb and exchange correlations helping explain the role of magnetic ordering in leading to gap formation in these novel complex oxides.

[1] B. J. Kim *et al.*, *Science* 323, 1329 (2009); B. J . Kim *et al.*, PRL 101, 076402 (2008).
[2] M. A. Laguna-Marco *et al.*, PRL 105, 216407 (2010); *ibid* PRB 90, 014419 (2014)
[3] D. Haskel *et al.*, PRL 109, 027204 (2012).

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