

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Crystal field splitting and correlation effect on the electronic structure of $A_2\text{IrO}_3$ HLYNUR GRETARSSON, J.P. CLANCY, University of Toronto, X. LIU, J.P. HILL, E. BOZIN, Brookhaven National Laboratory, Y. SINGH, Indian Institute of Science Education and Research Mohali, S. MANNI, P. GEGENWART, Georg-August-Universitat Gottingen, J. KIM, A.H. SAID, D. CASA, T. GOG, M.H. UPTON, Argonne National Laboratory, H.S. KIM, J. YU, Seoul National University, V.M. KATUKURI, L. HOZOI, J.V.D. BRINK, IFW Dresden, Y.J. KIM, University of Toronto — The electronic structure of the honeycomb lattice iridates Na_2IrO_3 and Li_2IrO_3 has been investigated using resonant inelastic x-ray scattering (RIXS). Crystal-field split $d-d$ excitations are resolved in the high-resolution RIXS spectra. In particular, the splitting due to non-cubic crystal fields, derived from the splitting of $j_{\text{eff}}=3/2$ states, is much smaller than the typical spin-orbit energy scale in iridates, validating the applicability of j_{eff} physics in $A_2\text{IrO}_3$. We also find excitonic enhancement of the particle-hole excitation gap around 0.4 eV, indicating that the nearest-neighbor Coulomb interaction could be large. These findings suggest that both Na_2IrO_3 and Li_2IrO_3 can be described as spin-orbit Mott insulators, similar to the square lattice iridate Sr_2IrO_4 .

Hlynur Gretarsson
University of Toronto

Date submitted: 26 Dec 2012

Electronic form version 1.4