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Report:

Motivated by recent theoretical calculations that predicted the realization of a pure (i.e. with perfect cubic symmetry) $J_{\text{eff}} = \frac{1}{2}$ state in Rb_2IrF_6[1], and therefore potential superconductivity in this sample if doped[2], we performed Resonant Inelastic X-ray Scattering (RIXS) measurements on this compound and other similar iridium fluorides (A_2IrF_6 and $BIrF_6$, where A = Li, Na, K, Cs and B = Sr, Ba). Ir L_3-edge RIXS has been extensively used in iridates as it is a direct probe of their electronic excitations, that are linked to the underneath ground state.

The collected RIXS spectra are shown in Fig. 1, where filled and empty circles are the spectra measured at 300 K and 10 K, respectively. Besides the elastic line, two features in the energy-loss range between 0.7 eV and 1.1 eV can be clearly seen. In accordance with other RIXS measurements on iridates, these features are assigned to transitions from the $J_{\text{eff}} = \frac{1}{2}$ to the $J_{\text{eff}} = \frac{3}{2}$ states. From the position of these two features, and with the help of a single-ion model that considers the effect of the spin-orbit coupling (ζ) and the trigonal contribution to the crystal field (Δ)[3], it is possible to estimate values of $\zeta \approx 0.6$ eV and $\Delta \approx -0.16$ meV for each compound. The value of the trigonal crystal field disagrees with previous theoretical calculations[1] and seems to indicate a larger departure from the cubic symmetry in Rb_2IrF_6 than in Sr_2IrO_4, which is the prototypical $J_{\text{eff}} = \frac{1}{2}$ Mott insulator.

The RIXS spectra show very little temperature dependence. Thus, the effective parameters of SOC and trigonal crystal field are not affected by temperature, at least in the range between 10 K and 300 K. The seemingly large change in the energy position of the $J_{\text{eff}} = \frac{3}{2}$ excitations in Na_2IrF_6 has been noticed to be caused by damage of the sample due to the beam exposure.
We are currently working on a publication on this subject.

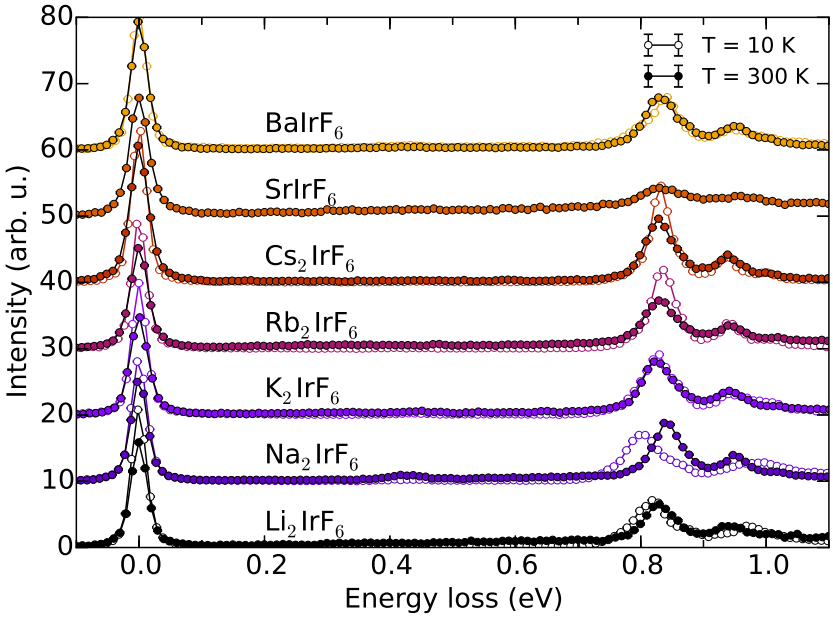

Figure 1: RIXS data of A_2IrF_6 (A = Li, Na, K, Rb, Cs) and $BIrF_6$ (B = Sr, Ba) at T = 10 K (empty circles) and T = 300 K (filled circles).

Bibliography:

[1] Birol and Haule, Phys. Rev. Lett. 114, 096403 (2015)
[2] Wang and Senthil, Phys. Rev. Lett. 106, 136402 (2011)
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