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Low energy excitations in iridates studied with Resonant Inelastic X-ray Scattering¹

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In the iridium oxides, the strong spin-orbit coupling (SOC) of the 5d iridium electrons entangles the orbital and spin degrees of freedom, providing opportunities for exotic magnetic states with highly anisotropic exchange interactions. At the same time, the spatially extended 5d electrons are expected to have much stronger hybridization with the oxygen 2p orbitals, comparing with that in 3d transition element compounds. Both factors make crystal symmetry and local environment crucial in determining the electronic and magnetic properties of the iridates. We present here our resonant inelastic X-ray scattering (RIXS) studies of a number of octahedrally coordinated iridates with special structures, exploring these effects. In particular, for the 1-D spin 1/2 chain compound, $\text{Sr}_3\text{CuIrO}_6$, the wavefunction of the hole in the t_{2g} manifold was reconstructed based on the RIXS spectra. Our results show that it is significantly modified from the isotropic shape expected for $J_{\text{eff}} = 1/2$ states in the strong SOC limit, due to the distortion of the oxygen octahedral cage. This distortion is comparable to, or smaller than, that present in most iridates and thus this work emphasizes the importance of local symmetry for the iridate families. Further, the magnetic excitations of this material were also measured. A large gap of ~ 30 meV, was found, comparable to the magnetic dispersion bandwidth. This is in contrast to the gapless dispersion expected for linear chain with isotropic Heisenberg exchange interaction. We also studied $\text{Na}_4\text{Ir}_3\text{O}_8$ which has a hyperkagome lattice, and is a candidate quantum spin liquid. Here, a low energy continuum is observed below the d-d excitations. Optical conductivity measurements performed on the same sample and polarization dependence of the RIXS signal suggest that these excitations are magnetic in origin, agreeing with the spin-liquid state prediction.

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