



	<b>Experiment title:</b> RIXS study of the metal-insulator transition $\text{Sm}_2\text{Ir}_2\text{O}_7$	<b>Experiment number:</b> HC-1976
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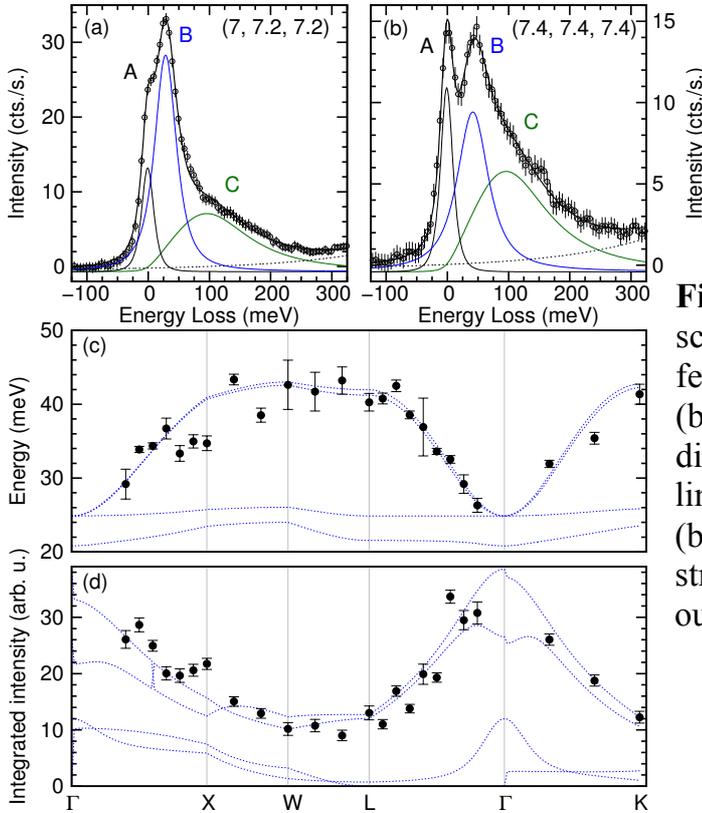
## Report:

We studied the magnetic and electronic excitations of the pyrochlore iridate  $\text{Sm}_2\text{Ir}_2\text{O}_7$  using resonant inelastic x-ray scattering (RIXS) at the Ir  $L_3$  edge. The electronic excitations within the  $t_{2g}$  manifold reveal that a large trigonal field exists that competes with the spin-orbit coupling (both  $\approx 400$  meV). We observed magnetic excitations at low temperature and were able to map out their dispersion across the entire Brillouin zone. The magnon dispersion is well-described by a Heisenberg exchange ( $J = 27.3(6)$  meV) and Dzyaloshinskii-Moriya interaction ( $D = 4.9(3)$  meV) and indicates strong electronic correlations.

The family of pyrochlore iridates,  $R_2\text{Ir}_2\text{O}_7$  (where  $R$  is a rare-earth element), has received much interest since the prediction of topologically non-trivial states, most prominently the Weyl semimetal [1–4]. This is motivated by the observation of metal-insulator transitions as a function of temperature and rare-earth ion radius that occur concomitantly with the onset of magnetic order. Despite substantial experimental effort, however, the nature of the magnetic order of the Ir ions and the effective spin Hamiltonian have remained elusive in pyrochlore iridates.

In this experiment we studied the magnetic and electronic excitations of  $\text{Sm}_2\text{Ir}_2\text{O}_7$  with RIXS. We were able to map out the magnon dispersion across the entire Brillouin zone. This presents a remarkable technical achievement, as a dispersion bandwidth of only 15 meV

could be observed. This demonstrates that RIXS at the iridium  $L_3$  edge can be used to study magnons at much lower energy scales than is currently known in literature. It promises to extend magnetic RIXS to many iridates other than the uniquely well-suited pervovskites  $\text{Sr}_2\text{IrO}_4$  and  $\text{Sr}_3\text{Ir}_2\text{O}_7$ , which offer magnon bandwidths of order 100 meV.



**Figure 1:** (a-b) Representative fitted RIXS energy scans of  $\text{Sm}_2\text{Ir}_2\text{O}_7$ . (c) Fitted energy dispersion of feature B as a function of momentum transfer (black dots) along with calculated magnon dispersion of all-in all-out order (blue dotted lines). (d) Fitted intensity dispersion of feature B (black dots) along with calculated total dynamical structure factor  $S(\mathbf{q}, \omega) = \sum_a S^{aa}(\mathbf{q}, \omega)$  of all-in all-out order (blue dotted lines).

Figure 1 shows the fitted magnon dispersion, using a Heisenberg exchange ( $J = 27.3(6)$  meV) and Dzyaloshinskii-Moriya interaction ( $D = 4.9(3)$  meV). One immediate result is that the dispersion is clearly gapped throughout the Brillouin zone, which is as expected for the proposed all-in all-out magnetic structure. The surprisingly “conventional” form of the magnetic Hamiltonian may be a direct consequence of the trigonal distortions (data not shown) that strongly degrade the idealised  $J_{\text{eff}}=1/2$  state towards a  $S=1/2$  doublet.

Furthermore, through comparison with published RPA calculations [5], we conclude that the magnon excitation spectrum is only compatible with a large Hubbard  $U$  limit. This is a non-trivial result, as most theory assumes a weak-to-intermediate coupling limit. At least for the case of  $\text{Sm}_2\text{Ir}_2\text{O}_7$ , this casts strong doubts on whether topological phases can be realized. Indeed, as even in the more metallic  $\text{Nd}_2\text{Ir}_2\text{O}_7$  clear charge gaps have been observed, electronic correlations may in general be too strong to realize novel topological phases in pyrochlore iridates – at least in the absence of external perturbations. The manuscript detailing this study is currently under review.

## References

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