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Report:

We examine the metal-insulator transition of the pyrochlore iridate $Nd_2Ir_2O_7$ with resonant inelastic x-ray scattering (RIXS). RIXS measurements were performed at the Ir L_3 edge (11.217 keV) to probe the magnetic and electronic excitiations of $Nd_2Ir_2O_7$ as a function of temperature, across the metal-insulator transition (MIT) at 40 K. The crystal-field excitations within the t_{2g} manifold show that trigonal distortions are as strong as the spin-orbit coupling in $Nd_2Ir_2O_7$, meaning that the electronic state deviates significantly from the J_{eff}=1/2 limit. The crystal-field excitations show little dependence on temperature, indicating that strong correlations persist in the high-temperature metallic state. Furthermore, we observe weakly temperature dependent, non-dispersive magnetic excitations at 60 meV energy loss.

The family of pyrochlore iridates, $R_2Ir_2O_7$ (R = rare-earth), show an MIT as a function of rare-earth ion radius [1]. This has lead to intriguing theoretical proposals of topologically non-trivial electronic states close to the MIT, such as the Weyl semi-metal [2-4]. $Nd_2Ir_2O_7$ is particularly interesting as it lies on the brink of the MIT, while still exhibiting an insulating, antiferromagnetic groundstate below 40 K. $Nd_2Ir_2O_7$ also hosts a thermal MIT at 40 K. The aim of the RIXS experiment was to characterize the magnetic and elecronic excitations below and above 40 K to address the MIT from a experimental point of view.

Figure 1 shows the RIXS map of $Nd_2Ir_2O_7$, collected in a low-resolution setup (360 meV). We identify transitions within the t_{2g} manifold and to the e_g manifold resonating 3 eV apart, which provides a rough estimate of the cubic crystal field. In order to effectively promote transitions to the t_{2g} states, we set the incident energy to 11.214 keV.

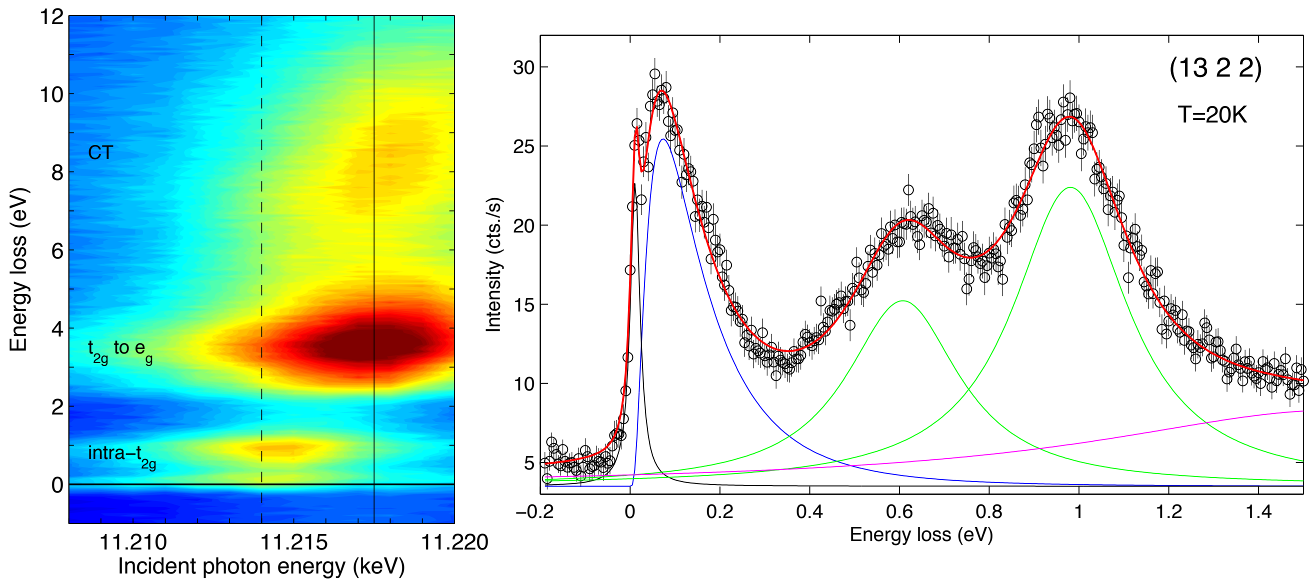
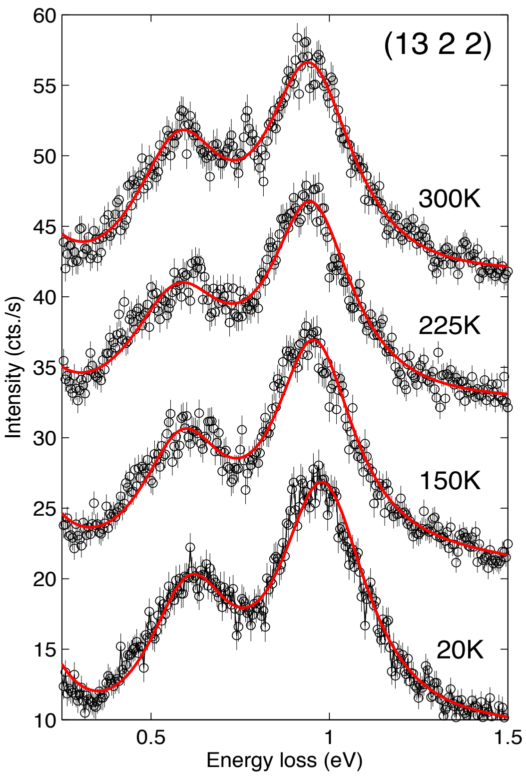


Figure 1: *Left:* Low energy resolution (360 meV) RIXS map of $Nd_2Ir_2O_7$. *Right:* High energy resolution (26 meV) energy scan of $Nd_2Ir_2O_7$ at **Q** = (13 2 2) at 20 K, showing crystal field excitations (0.6 eV and 1 eV) and magnetic excitations (60 meV).

In the high-resolution energy scan at **Q** = (13 2 2) at 20 K, we identify intra-t_{2g} excitations at 0.6 eV and 1 eV. For an ideal J_{eff}=1/2 state only a single excitation is expected. The presence of two excitations can be explained within a single-ion model that includes spin-orbit coupling and trigonal distortions. Within this model, we estimate the strength of the spin-orbit coupling and trigonal distortions as 460 meV and 490 meV, respectively. This implies that the electronic ground state lies halfway between a J_{eff}=1/2 and a "regular" S=1/2 doublet.

We also observe an excitation at 60 meV energy loss. This feature is weakly temperature dependent and we assign a magnetic origin to it. However, within the experimental resolution we could not detected any momentum dispersion. The absence of dispersion may indicate a highly anisotropic magnetic Hamiltonian for $Nd_2Ir_2O_7$, but further investigations are required.



We also studied the temperature dependence of RIXS excitations. Figure 2 shows the crystal-field excitations within the t_{2g} manifold as a function of temperature. Across the thermal MIT at 40 K, little change is seen. Indeed, up to room temperature, the energy of the excitations and their width stays remarkably unchanged. The first implies that trigonal distortions are not driving the MIT. The second means that even at highest temperatures there are strong correlations and the local moment character persists. Below 40 K, at the magnetic transition, these preformed moments order and an electronic gap opens.

Figure 2: Temperature dependence of crystal-field excitations within the t_{2g} manifold of $Nd_2Ir_2O_7$.

References

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