



**Experiment title:**

Elementary excitations in the quasi-1D dimer-chain iridate  $\text{Ba}_5\text{AlIr}_2\text{O}_{11}$

**Experiment number:**

HC-2566

**Beamline:**

**Date of experiment:**

from: 13.04.2016 to: 19.04.2016

**Date of report:**

05.09.2016

**Shifts:**

**Local contact(s):**

Marco Moretti Sala

*Received at ESRF:*

**Names and affiliations of applicants** (\* indicates experimentalists):

Xingye Lu, D. E. McNally, T. Schmitt

Department of Synchrotron Radiation and Nanotechnology, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland

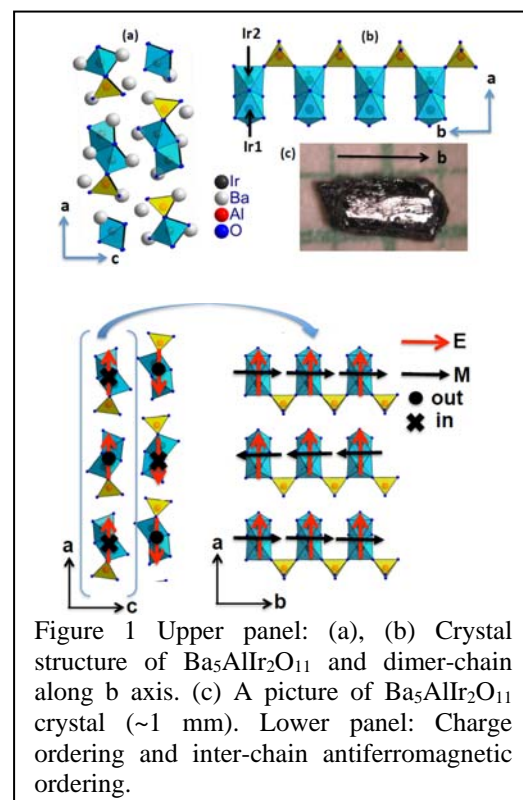
**Report:**

We have carried out resonant inelastic X-ray scattering (RIXS) experiment ‘Elementary excitations in the quasi-1D dimer-chain iridate  $\text{Ba}_5\text{AlIr}_2\text{O}_{11}$ ’ (proposal HC-2566) on ID20 of ESRF. We find that the quasi-1D dimer chain  $\text{Ba}_5\text{AlIr}_2\text{O}_{11}$  bearing mixing valence states ( $\text{Ir}^{4+}$  and  $\text{Ir}^{5+}$ ) [1] shows much more complicated crystal field excitations than typical  $\text{Ir}^{4+}$  systems, which is caused by electronic transitions between the electronic levels within  $t_{2g}$  orbitals of the molecular clusters.

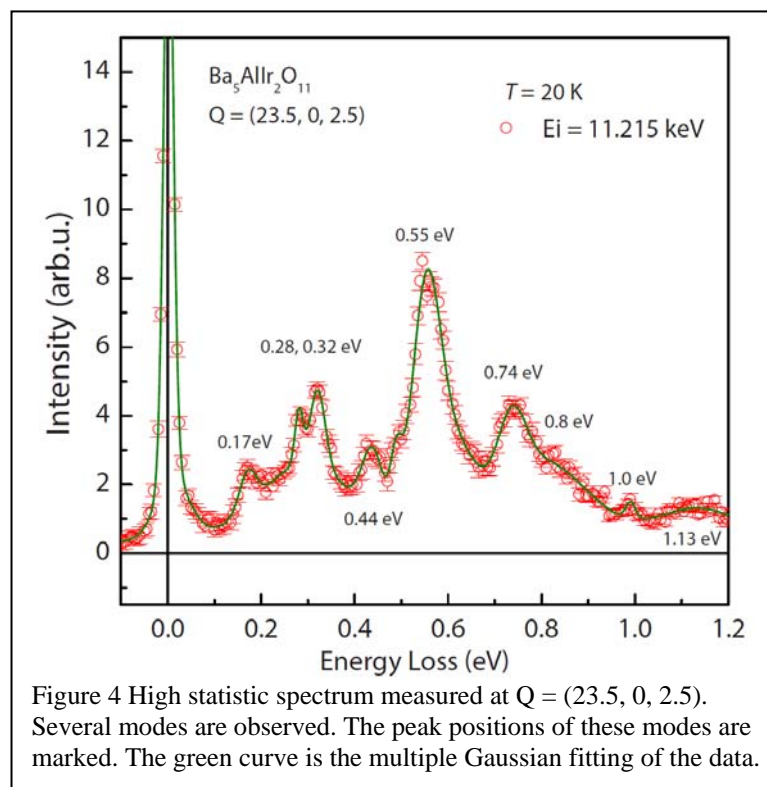
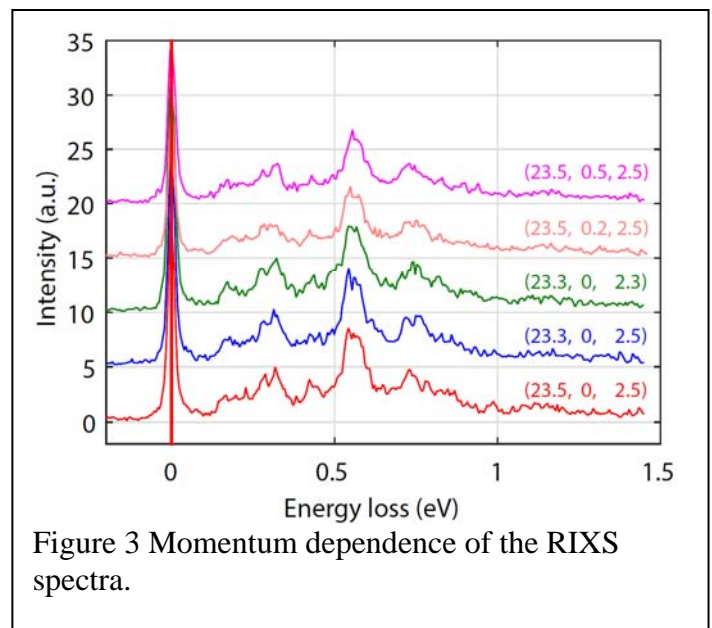
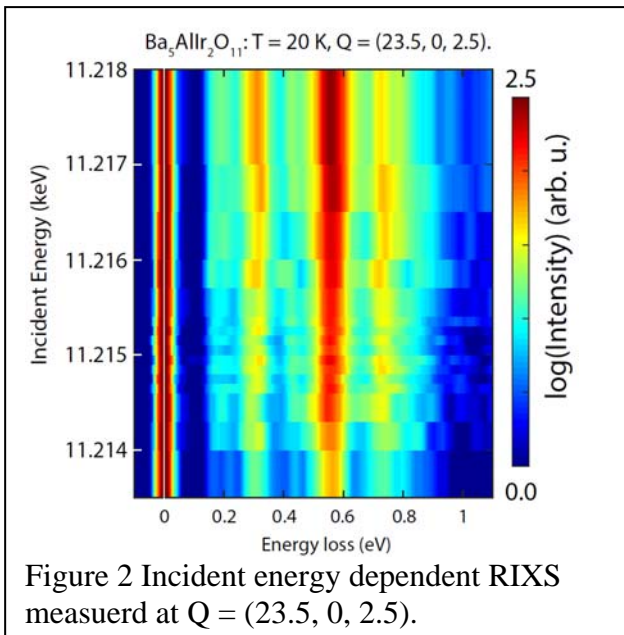
$\text{Ba}_5\text{AlIr}_2\text{O}_{11}$  consists of dimer-chains lying along the  $b$  axis, with the dimers containing two face-sharing  $\text{IrO}_6$  octahedra, which are weakly connected by  $\text{AlO}_4$  tetrahedra, while the dimer-chains are well separated. This structure characteristically generates weak intra-chain interactions between dimers and even weaker inter-chain couplings. The system shows different local distortions for  $\text{Ir1-O}$  and  $\text{Ir2-O}$  octahedra, with slight differences in the Ir-O bond length, indicating a more complicated non-cubic crystal electric field within the isolated dimer [1].

The incident energy dependent RIXS spectra shown in Fig. 2 reveals various Raman modes corresponding to low energy crystal field excitations within  $t_{2g}$  orbitals, ranging from  $\sim 0.2\text{eV}$  to  $\sim 1.3\text{eV}$ . We have also observed  $t_{2g}-e_g$  transitions at  $\sim 3\text{eV}$  (not shown here). These Raman modes within  $t_{2g}$  orbitals are quite narrow in energy and not followed by any fluorescence. Moreover,  $\text{Ba}_5\text{AlIr}_2\text{O}_{11}$  is a strong Mott insulator, indicative of a large insulating gap. Therefore, we attribute these Raman modes to the local modes arising from the transitions between the electronic levels within  $t_{2g}$  orbitals of the dimer molecular clusters.

As a result of the difference in local distortion and underlying electronic interactions, the system shows partial charge disproportion ( $\text{Ir1}$  is closer to  $\text{Ir}^{5+}$  and  $\text{Ir2}$  to  $\text{Ir}^{4+}$ ), indicative of a charge order (below 210 K). However, our momentum dependent RIXS measurements shown in Fig. 2 do not show any collective excitations. All the Raman modes we observed are dispersiveless (local modes). This could be ascribed to the weak electronic interactions between the dimers.



To quantitatively determine the crystal field excitations shown in Fig. 2 and 3, we have performed high statistic RIXS measurements at  $Q = (23.5, 0, 2.5)$ . The spectrum and its fitting by multi-gaussians are shown in Fig. 4. About 10 Raman modes have been identified between 0.1eV and 1.2eV, indicating that rich electronic levels are formed in the  $t_{2g}$  orbitals of this system. No modes were observed between 1.2eV and  $t_{2g}$ - $e_g$  transitions. Quantitative analysis of the microscopic origin of these low energy crystal field excitations are still in progress.



#### Reference:

[1] J. Terzic *et al.*, Phys. Rev. B **91**, 235147 (2015).