ESRF	Experiment title: Electronic ground state in the ideal $J_{\text{eff}} = \frac{1}{2} \text{ Rb}_2 \text{IrF}_6$ investigated by combined F K-edge RIXS and XAS study	Experiment number: HC 2710
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Report:

The search for SU(2) invariant $J_{\text{eff}} = \frac{1}{2}$ quantum states is boosted by theoretical predictions of superconductivity in these systems when doped [1]. Sr₂IrO₄ is the model $J_{\text{eff}} = \frac{1}{2}$ material [2], and it has been intensively studied in the last decade. However, no superconductivity has been detected so far, probably because of the symmetry breaking induced by the local octahedral distortion. Recently, much attention has been put on iridium fluorides [3], since theoretical studies propose them as the closest systems to the SU(2) symmetric $J_{\text{eff}} = \frac{1}{2}$ state [4]. In particular, Rb₂IrF₆ has the K₂GeF₆ crystal structure (space group P-3m1) where the IrF₆ octahedra are all isolated and present a small trigonal distortion. The aim of this experiment is to obtain informations about the ground state symmetry of Rb₂IrF₆ by probing the ligand states, as already done by some of the authors in Ba₂IrO₄ [5]. This gives quantitative informations about the spin-orbit coupling and crystal field.

The F K-edge XAS spectrum is reported in Fig. 1(a). Due to several sample charging issues, the only way we could measure the electron yield was to press powder of Rb_2IrF_6 into an indium foil to enhance the conductivity of the system. Thus, we could not exploit the polarization dependence of the XAS spectrum to gain informations about the orbital occupancies, as was initially planned. However, we can assign the first peak at 682.4 eV to the transition of an electron from the F 1s to the F 2p orbitals which are mixed with the Ir t_{2g} states, while the second peak at 684.6 eV is ascribed to the transition of an electron from the F 2p orbitals mixed with the Ir e_g states.

Indeed, the RIXS spectrum measured with incident photon energy of 682.4 eV (Fig. 1(b)) shows the presence of a weak feature at energy loss of 0.9 eV. This feature is absent in the RIXS spectrum measured with incident photon energy of 684.6 eV. Therefore, we ascribe this feature to intra- t_{2g} excitations, in agreement with the Ir L₃-edge RIXS spectrum of Rb₂IrF₆ [6]. The intense feature at higher energy losses in the RIXS spectrum (Fig. 1(b)) has the characteristics of resonant fluorescence emission, as verified by inspecting their incident photon energy dependence.



Figure 1: (a) F K-edge XAS spectrum of Rb_2IrF_6 for photons impinging on the sample at normal incidence. (b) F K-edge RIXS spectrum of Rb_2IrF_6 measured with an incidence angle of 45° (specular geometry).

Bibliography:

- [1] F. Wang and T. Senthil, Phys. Rev. Lett. 106, 136402 (2011)
- [2] B. J. Kim et al., Phys. Rev. Lett. 101, 076402 (2008)
- [3] K. S. Pedersen et al., Nat. Comm. 7, 12195 (2016)
- [4] T. Birol and K. Haule, Phys. Rev. Lett. 114, 096403 (2015)
- [5] M. Moretti Sala et al., Phys. Rev. B 89, 121101(R) (2014)
- [6] M. Rossi et al., ESRF Experiment report HC-2571 (2016)