# RIXS of CuFeO2: Probing the band structure of a copper-based semiconductor as a gateway into the RIXS cross-section for cuprates

Jason HANCOCK[1] Guillaume CHABOT-COUTURE[1] Kenji ISHII[2] Ignace JARRIGE[2]
Noriki TERADA[3] Martin GREVEN[1]
1)Stanford University 2)JAEA, SPring-8 3)NIMS, Tsukuba

Detailed measurements of the charge-transfer excitations in the 1-10 eV range were performed on the copper based semiconductor CuFeO2 using resonant inelastic X-ray scattering (RIXS). The momentum dependence, scattering geometry dependence, and the incident energy dependence were investigated.

Keywords: CuFeO2, RIXS, charge-transfer, x-ray, momentum-resolved, polarization

## 1. Purpose

We characterized the band structure of CuFeO2 using resonant inelastic X-ray scattering. This band insulator is a very important compound due to its transparent nature. Using RIXS at the Cu *K*-edge, it is possible to measure the band dispersion as well as the direct and indirect band gaps of this delafossite. In addition, we carry out a careful incident energy and scattering geometry dependent study of the cross-section to elucidate the properties of RIXS as an experimental technique.

## 2. Method

To establish the resonance profile of this system, we measured complete incident energy dependence over both the in-plane and the out-of-plane resonances on a fine grid. At the most intense feature, we measured detailed momentum dependence and constructed a dispersion diagram along the high-symmetry directions of the Brillouin zone. To study the internal details of the RIXS cross-section but also of the measured excitations, we looked into scattering geometry dependence, i.e., the combined effects of incident and outgoing photon polarization.

## 3. Result

The incident energy dependence of the RIXS spectra reveals at least four distinct electronic excitations at the zone center. Theoretical studies of the electronic structure [1] show that the Cu *3d*, the Fe *3d*, and the O *2p* states are within a few eV of the Fermi level and should take part in the observed inter-band transitions. By measuring the momentum dependence of the lowest electronic excitations, we observed both direct and indirect gaps and a clear dispersion of the lowest two inter-band transitions. The lowest-energy feature, at 2 eV, disappears rapidly away from the zone center, suggesting that it is excitonic in nature. The highest-energy excitation is independent of momentum transfer and has an energy-loss value of twice (11eV) the second lowest inelastic feature at 5.5 eV. This suggests that it could consist of the creation of two electron-hole pairs, each with 5.5 eV on average. Measurements of the dispersion of excitations along the *L*-direction also show a very weak dependence which suggests that the excitations are essentially two-dimensional in nature. Finally, we found that the scattering geometry dependence of the inelastic spectrum is consistent with the '4*p*-as-spectator' approximation of the 'indirect' RIXS cross section.

## 4. Conclusion

We have characterized the momentum and incident energy dependence of the RIXS spectrum of the copper-based semiconductor CuFeO2. We observed distinct inelastic features and characterize their dispersion. We expect our measurements of CuFeO2 to generate interest beyond the RIXS community, to lead to a better understanding of the electronic structure of this delafossite, and to improve our understanding of the RIXS cross section as well.

## 5. Reference

[1] V. R. Galakhov, A. I. Poteryaev, E. Z. Kurmaev, V. I. Anisimov, St. Bartkowski, M. Neumann, Z. W. Lu, B. M. Klein, and Tong-Rong Zhao, Phys. Rev. B **56**, 4584 (1997)