Resonant inelastic x-ray scattering of strongly correlated copper oxides

Jason Hancock[1)], Guillaume Chabot-Couture[1)], Martin Greven[1)],
Kenji Ishii[2)], Jun'ichiro Mizuki[2)], Guerman Petrakovskii[3)]

[1)]Stanford University, California, USA, [2)]JAEA, [3)]Kirenskii Institute, Krasnoyarsk, Siberia

We performed a detailed study of the Cu K-edge resonant inelastic x-ray scattering (RIXS) response of CuB_2O_4, an insulating system that represents the simplest possible electronic structure of cuprate oxides, with covalently bonded CuO_4 units separated by B^{+3} ions.

Keywords : resonant inelastic x-ray scattering, strongly correlated electron systems

1. Purpose

Most previous experimental work has focused on electronically complex systems such as the 2D lamellar cuprate systems. CuB_2O_4, however is a quasi-zero dimensional cuprate oxide: the lattice structure suggests that the Cu and O related electronic structure may be envisioned as an effective gas of isolated CuO_4 plaquettes which do not pass charge. The electronic structure of this system is relatively simple, and so constitutes an ideal candidate for developing generalizable notions of the RIXS technique which is computationally tractable.

2. Method

RIXS Spectra were taken at the JAEA beamline BL11XU at SPring8 in a horizontal scattering geometry with the incident (horizontal) beam polarization along the tetragonal c axis, near a momentum point (9,0,4), with a scattering angle $2\theta \sim 93°$. The overall energy resolution was around 380 meV.

3. Result

We obtained two full contour plots (incident energy versus energy transfer versus signal) and angle-dependent scans as well as several line scans to explore momentum dependence. Several prominent features appear at 1.9 eV, 6.75 eV, and 10.9 eV. As was suggested in the context of Li_2CuO_2 [1], we conclude that the 1.9 eV feature represents a local d-d excitation. The 6.75 eV feature is perhaps the most prominent Raman feature, and in accord with previous work, we assign the majority of the spectral weight in this region to the molecular orbital (MO) excitation [2]. Contrary to the d-d excitation which resonates strongly near two distinct energies, 8992 eV and 8998 eV, the MO excitation shows as a long streak, with center shifts that depend strongly on incident energy. From a cluster calculations, we find that RIXS processes with 4p final states are likely sources for the high energy excitation at 10.9 eV [3].

4. Conclusion

We studied charge excitations of CuB_2O_4 by RIXS technique. Three excitations at 1.9 eV, 6.75 eV, and 10.9 eV are observed in the spectra, which are assigned to the local d-d excitation, the molecular orbital excitation, and the excitation to 4p final state, respectively.

5. Reference

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