

Theoretical and Experimental Investigations of Cu K α Resonant X-ray Emission Spectra for La₂CuO₄ ---- An Ultra-fine Probe for the Pre-edge Structure of Cu 1s Electron Excitation -----

A. Kotani^{1,2}, M. Taguchi¹, K. Okada³, M. Calandra⁴ and A. Shukla⁴

¹*Soft X-ray Spectroscopy Laboratory, RIKEN/Spring-8
1-1-1 Kouto, Mikazukicho, Sayo, Hyogo 679-5148, Japan*

²*Photon Factory, IMSS, High Energy Accelerator Research Organization
Tsukuba, Ibaraki 305-0801, Japan*

³*The Graduate School of Natural Science and Technology, Okayama University, 3-1-1
Tsushima-naka, Okayama 700-8530, Japan*

⁴*Laboratoire de Minéralogie de Paris, 4 Place Jussieu, 75252, Paris cedex 05, France*

X-ray absorption is the standard method to probe the unoccupied density of states (DOS) at a given edge. Here we show that polarized Resonant X-Ray Emission Spectroscopy (RXES) in La₂CuO₄ at the Cu K-edge is extremely sensitive to the environment of the Cu atom and the fine structure in the Cu 4p DOS. Calculations combining *ab initio* SPGGA+U (Spin-polarized generalized gradient approximation + on-site U) method with a many-body cluster model including a single Cu site, used for the first time in such a context, show remarkable agreement with experiment. In particular, we show that an extremely weak *off-site* Cu 1s-3d dipole transition mediated by Cu 4p-O 2p and O 2p-Cu 3d hybridizations and never before identified can also be clearly detected by the Cu K α RXES [1]. We also perform a multi-Cu-site cluster model calculations of the Cu K α RXES, where the effects of non-local screening and non-local dipole transition are explicitly taken into account [2].

[1] A. Shukla, M. Calandra, M. Taguchi, A. Kotani, G. Vanko and S.-W. Cheong, preprint.

[2] K. Okada and A. Kotani, unpublished.