

Abstract Submitted  
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**Ab initio calculation of d-metal L-edge RIXS spectra using many-body quantum chemistry methods** NIKOLAY BOGDANOV, Institute for Theoretical Solid State Physics, IFW Dresden, Germany, VALENTINA BISOGNI, Paul Scherrer Institut, Villigen, Switzerland, JOCHEN GECK, Institute for Solid State Research, IFW Dresden, Germany, LIVIU HOZOI, JEROEN VAN DEN BRINK, Institute for Theoretical Solid State Physics, IFW Dresden, Germany — We designed a fully ab initio quantum chemistry scheme for the computation of both d-d excitation energies and intensities as measured by resonant inelastic x-ray scattering (RIXS) in d-electron systems. RIXS has recently emerged as a powerful tool to reliably probe the charge, spin, and orbital degrees of freedom of correlated electrons in solids [1,2]. As a first application we picked up  $\text{Li}_2\text{CuO}_2$ , a quasi-1D Cu  $3d^9$  oxide with a simple valence configuration in the intermediate state. We use embedded-cluster MCSCF and MRCI techniques [3], including scalar relativistic effects, spin-orbit coupling, and the valence orbital relaxation in the presence of the core hole. The transition matrix elements of the dipole operator are obtained by non-orthogonal configuration interaction. A careful analysis of the RIXS spectra is important for understanding the interplay between local distortions and longer-range lattice anisotropy and its effect on the d-level electronic structure [3,4] and magnetic interactions [4]. [1] L. Ament *et al.* Rev. Mod. Phys. **83**, 705 (2011); [2] J. Schlappa *et al.* Nature **485**, 82 (2012); [3] H.-Y. Huang *et al.* Phys. Rev. B **84**, 235125 (2011); [4] N. A. Bogdanov *et al.* Phys. Rev. Lett. **110**, 127206 (2013).

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