Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Real-time cumulant approach for inelastic losses in x-ray spectra[1]

J. J. KAS, J. J. REHR, U of Washington, J. B. CURTIS, U of Rochester — Intrinsic inelastic losses in core level x-ray absorption (XAS), emission (XES), and x-ray photo-emission spectra (XPS), arise from excitations of the system due to the sudden creation or annihilation of a deep core hole. Additional extrinsic losses arise during the propagation of the photoelectron, and interference processes are also important. These excitations are reflected in the satellite peaks observed in XPS. Formally the distribution of these excitations are described in terms of the core-hole spectral function, which can be calculated in terms of the core-hole Green's function represented in exponential form. Here we discuss an approach for calculating the exponent, or cumulant in terms of local density fluctuations via real-space, real-time time-dependent density functional theory.[2] The role of extrinsic and interference terms is also discussed. Our method is illustrated in calculations of XAS and XPS for number of systems, including weakly correlated as well as d- and f-electron materials.

[1]Supported by DOE BES Grant DE-FG03-97ER45623

[2]J. J. Kas, F. D. Vila, J. J. Rehr, and S. A. Chambers, Phys. Rev. B **91**, 121112 (2015).

J. J. Kas
U of Washington

Date submitted: 04 Nov 2015 Electronic form version 1.4