

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Real-time calculations of dynamical effects in x-ray spectra**<sup>1</sup> J.J. REHR, J.J. KAS, A.J. LEE, Univ of Washington — An understanding of dynamical effects and inelastic losses in x-ray spectra due to the sudden creation of a core-hole and photoelectron has long been of interest. Here we present a real-time approach for calculations of core level x-ray absorption and x-ray photoemission spectra that account for the dynamic response in terms of a spectral function that includes intrinsic, extrinsic and interference terms. Our approach is based on a factorization in terms of the core-hole Green's function and a time-correlation function that avoids the need for ultra-short time-steps. The approach extends a time-correlation function approach for XAS,<sup>2</sup> and a real-time TDDFT approach for XPS.<sup>3</sup> The approach permits a real-space picture of many-body excitations such as satellites and inelastic losses analogous to that for XPS. The method is implemented using an adaptation of the Crank-Nicholson time-evolution algorithm with PAW transition matrix elements. Illustrative examples are presented for a number of systems.

<sup>1</sup>Supported by DOE BES DE-FG03-97ER45623.

<sup>2</sup>A. J. Lee, F. D. Vila and J. J. Rehr, Phys. Rev. B **86**, 115107 (2012)

<sup>3</sup>J. J. Kas, F. D. Vila, J. J. Rehr, and S. A. Chambers, arXiv:1408.2508

John Rehr  
Univ of Washington

Date submitted: 14 Nov 2014

Electronic form version 1.4