

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Bethe-Salpeter Equation calculations of transition metal  $L_{2,3}$  edge x-ray spectra including multiplet effects**<sup>1</sup> J. VINSON, U. Washington, E.L. SHIRLEY, NIST, J.J. REHR, U. Washington — Calculations of x-ray spectra at transition metal  $L_{2,3}$  edges often present theoretical difficulties due to strong core-hole multiplet effects. Here we discuss an *ab initio* method for treating these effects following the Bethe-Salpeter Equation (BSE) approach of Shirley.<sup>2</sup> The method builds in spin-orbit interactions, intra-atomic Coulomb integrals, core-hole screening, and band-structure effects, and thus accounts for multiplet effects without the need for phenomenological ligand-field parameters. The method has been implemented in the core-level BSE code OCEAN,<sup>3</sup> which uses as input wavefunctions from planewave, pseudopotential DFT calculations and PAW transition matrix elements. Examples are presented for several transition metal systems and compared with experiment.

<sup>1</sup>Supported by DOE BES DMSE Grant DE-FG03-97ER45623 and facilitated by the DOE CMCSN

<sup>2</sup>E. L. Shirley, *J. Electron Spectrosc. Relat. Phenom.* **144**, 1187 (2005).

<sup>3</sup>J. Vinson, E. L. Shirley, J. J. Rehr, and J. J. Kas, arXiv:1010.0025

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Date submitted: 22 Dec 2010

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