

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Large-scale Bethe-Salpeter equation calculations of core-level x-ray spectra¹ J. J. REHR, J. VINSON², K. GILMORE, U. Washington — Recently an approach has been developed for Bethe-Salpeter equation (BSE) calculations of core-level x-ray spectra, which is implemented in the OCEAN package ³ which combines plane-wave, pseudopotential DFT electronic structure, PAW transition elements, GW self-energy corrections, and the NIST BSE solver. The method yields both dipole limited and finite momentum transfer spectra. Here we discuss several recent advances which yield a unified treatment of both extended states and atomic multiplet effects. In particular our approach now includes spin-dependent potentials and hole-dependent lifetimes, and gives an improved treatment of L_{2,3} edges, where contributions to spectral weight come from a mix of two distinct core holes. We have also extended the code interface to include pseudopotential wave functions from ABINIT, QUANTUMESPRESSO, or an interpolation based scheme, thus enabling large-scale calculations with unit cells in excess of 2000 Å³. Applications to water and ice structures are briefly discussed.

¹Supported by DOE BES Grant DE-FG03-97ER45623 and facilitated by the DOE CMCSN

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Date submitted: 08 Nov 2012

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