Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Obtaining core excitation spectra using ABINIT and NBSE[1]
JOHN VINSON, U. of Washington, ERIC SHIRLEY, NIST, JOHN REHR, JOSHUA KAS, U. of Washington — We present a hybrid approach for GW/Bethe-Salpeter Equation calculations of core excitation spectra including XAS, NRIXS and EELS. The method dubbed OCEAN, is based on 1) *ab initio* ground state wavefunctions from the plane-wave pseudopotential code ABINIT; 2) the NIST core-level Bethe-Salpeter Equation Lanczos solver; and 3) a many-pole GW self-energy model (MPSE) to approximate final state broadening and self-energy shifts. An easy to use interface has been developed to drive the different steps required. Extensions to related spectra are briefy discussed. Examples are presented for the F and Li K-edge XAS in LiF, the O K-edge in ice-1h, and others.

[1]Supported by DOE BES Grant DE-FG03-97ER4523.

John Vinson
U. of Washington

Date submitted: 20 Nov 2009 Electronic form version 1.4