Bethe-Salpeter equation calculations of resonant inelastic x-ray scattering at the nitrogen K edge JOHN VINSON, TERRENCE JACH, NIST, Gaithersburg, MD, TIM ELAM, Applied Physics Laboratory, U. Washington, JONATHON DENLINGER, Advanced Light Source, LBL — We present theoretical calculations of resonant inelastic x-ray scattering (RIXS) at the nitrogen K edge of several materials along with direct comparison to experimental results. Our approach is based on a Bethe-Salpeter equation formalism, and our calculations are carried out using an extension of the OCEAN package,[1] including both intermediate and final-state excitonic effects. By building upon a DFT basis we include ground-state effects without system-dependent fitting parameters. We are able to account for the general trends and features seen in experiment. A more *ad hoc* account of other contributions to the measured spectra, primarily phonon coupling, is attempted, but this highlights some current shortcomings limiting fully *ab initio* calculations of the near-edge x-ray spectra of extended systems.

[1] J. Vinson, E. L. Shirley, J. J. Rehr, and J. J. Kas, Phys. Rev. B **83**, 115106 (2011)

John Vinson
NIST, Gaithersburg, MD

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