

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

RIXS of Ammonium Nitrate using OCEAN JOHN VINSON, TERENCE JACH, NIST, Gaithersburg, MD, MATTHIAS MUELLER, RAINER UNTERUMSBERGER, BURKHARD BECKHOFF, PTB, Berlin, Germany — The OCEAN code allows for calculations of near-edge x-ray spectroscopies using a *GW*/Bethe-Salpeter equation (BSE) approach. Here we present an extension of the code for calculating resonant inelastic x-ray scattering (RIXS). Recent work has shown that peak-specific broadening of nitrogen $K\alpha$ emission in nitrates is due to a valence-band lifetime that is an order of magnitude shorter than that of the nitrogen $1s$ hole, an inversion of the usual assumption that valence holes have longer lifetimes than core-level holes. Using the BSE, including *GW* corrections to the DFT energies, as implemented in OCEAN we are able to compare calculations of RIXS with measured spectra of the same. By utilizing an approach free from fitting parameters we are able to identify the origins of various broadening effects observed in experiment.

John Vinson
NIST, Gaithersburg, MD

Date submitted: 03 Nov 2015

Electronic form version 1.4