Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First principles calculations of optical and x-ray spectra from atomic coordinates alone[1] J.J. KAS, M. PRANGE, F.D. VILA, Y. TAKIMOTO, J.J. REHR, University of Washington — Theoretical calculations of various x-ray and optical spectroscopies often rely on semi-empirical or phenomenological models to account for many-body effects and thermal vibrations. Typically such models include a number of parameters which complicate fitting schemes that extract physical quantities from experimental spectra. Here we present an approach for *ab initio* calculations of these spectra starting from structure alone. A many-pole model of the dielectric function is introduced to calculate the self-energy and spectral function,[2] while a density functional theory calculation of the dynamical matrix is used to calculate effects of thermal vibrations. [3] In addition, core-hole effects are incorporated with RPA screening. [4] This approach has been incorporated into FEFF9, a new version of the real-space multiple-scattering FEFF code for broad spectrum calculations of various optical and x-ray spectra.

[1]Supported by DOE Grant DE-FG02-97ER45623 (JJR and MP), NIH NCRR BTP grant RR-01209 (JK), NSF 0120967 (YT).
[2]J. J. Kas et al., Phys. Rev. B **76** 195116 (2007).
[3]Fernando D. Vila et al., Phys. Rev. B **76**, 014301 (2007).
[4]A. L. Ankudinov et al., Phys. Rev. B **71**, 165110 (2005).

Joshua Kas
University of Washington

Date submitted: 01 Dec 2007 Electronic form version 1.4