Real Space Green's Function Theory of X-ray Absorption and Electron Energy Loss Spectra

J. J. Rehr

Department of Physics, University of Washington
Seattle, WA, USA

There has been substantial progress in recent years in theories of x-ray absorption (XAS) and electron energy loss spectra (EELS).[1] A major challenge for the theory is that such spectra reflect the excited state electronic structure in a material. Thus calculations must take into account such many-body effects as inelastic losses and core-hole screening. Our approach is based on the real-space Green's function (RSGF) method which widely used for calculating such spectra.[2] We begin with an independent, quasi-particle approximation, which builds in the most important many-body effects. In particular the final states are calculated with a complex self-energy to account for inelastic losses. Our self-energy is obtained using the GW approximation and a many-pole model for the dielectric response function.[3] Local fields and core-hole screening are treated using a combination of time-dependent density functional theory (TDDFT) and the Bethe-Salpeter equation (BSE). Intrinsic losses are obtained using a quasi-boson method and a generalization of the GW approximation. Finally, Debye-Waller factors are calculated using a Lanczos algorithm and an *ab initio* dynamical matrix from ABINIT. With these techniques we obtain ab initio XAS, EELS and NRIXS[4] spectra over a broad spectrum without adjustable parameters. This work is supported by DOE Grant DE-FG03-97ER45623 and facilitated by the DOE CMSN.

[1] J. J. Rehr and R. C. Albers, Rev. Mod. Phys. 72, 621 (2000).

[2] A. L. Ankudinov, J. J. Rehr and Y. Takimoto, Phys. Rev. B 71, 165110 (2005).

[3] A. P. Sorini, J. J. Kas, J. J. Rehr, M. P. Prange and Z. H. Levine, Phys. Rev. B **74**, 165111 (2006).

[4] J. A. Soininen, A. L. Ankudinov, and J. J. Rehr, Phys. Rev. B 72, 045136 (2005).