Abstract Submitted
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***Ab initio* calculations of intrinsic and extrinsic losses in x-ray spectra**[1] J. KAS, M. PRANGE, J. J. REHR, U. of Washington, L. W. CAMPBELL, PNNL, J. A. SOININEN, U. of Helsinki — Typical calculations of x-ray absorption spectra (XAS) include inelastic losses within the quasi-particle approximation, which neglects satellite structure in the spectral function. While satellite effects are relatively small in the EXAFS region, they can be quite large for near edge spectra. Here we present an efficient *ab initio* approach for calculating inelastic losses due to both intrinsic and extrinsic many body interactions, as well as interference between them. The method begins with a real-space multiple-scattering calculation of the dielectric function $\epsilon(\omega)$,[2] which is then fit to a many-pole model with approximately 10^2 poles. This yields a many-pole approximation to GW self-energies, as well as a many-pole spectral function, and estimates for the many-body amplitude factor in XAS. Results for the self-energy agree well with other calculations.[3] The approach also gives improved agreement for core-level XAS, especially in the near edge region.

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[2]J.J. Rehr et al., cond-mat/0601241 (2006)
[3]J.A. Soininen et al., J. Phys. Condens. Matter. 15 (2003)

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