Abstract Submitted
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***Ab initio* Quasiparticle Self-Energies and X-ray spectra**[1] J. KAS, M. PRANGE, A. SORINI, J.J. REHR, U. of Washington — Present calculations of inelastic losses in x-ray spectra typically employ semi-empirical or highly simplified models, such as the plasmon-pole self-energy, which are only semi-quantitative for near edge spectra. Here we present an efficient *ab initio* approach applicable to general materials, starting from a real-space multiple-scattering calculation of the dielectric function,[2] which is fit to a multiple-pole model with of order 10^2 poles. This yields multiple-pole GW self-energies, and hence related quantities such as inelastic mean free paths (IMFP). The approach leads to improved amplitudes and phases for core-level x-ray spectra up to photo-electron energies of order 10^3 eV. Results for the IMFP are found to be in good agreement with experiment and with other approaches.[3,4]

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