Real-time calculations of dynamical effects in x-ray spectra\textsuperscript{1} J.J. REHR, J.J. KAS, A.J. LEE, Univ of Washington — An understanding of dynamical effects and inelastic losses in x-ray spectra due to the sudden creation of a core-hole and photoelectron has long been of interest. Here we present a real-time approach for calculations of core level x-ray absorption and x-ray photoemission spectra that account for the dynamic response in terms of a spectral function that includes intrinsic, extrinsic and interference terms. Our approach is based on a factorization in terms of the core-hole Green’s function and a time-correlation function that avoids the need for ultra-short time-steps. The approach extends a time-correlation function approach for XAS,\textsuperscript{2} and a real-time TDDFT approach for XPS.\textsuperscript{3} The approach permits a real-space picture of many-body excitations such as satellites and inelastic losses analogous to that for XPS. The method is implemented using an adaptation of the Crank-Nicholson time-evolution algorithm with PAW transition matrix elements. Illustrative examples are presented for a number of systems.

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\textsuperscript{3}J. J. Kas, F. D. Vila, J. J. Rehr, and S. A. Chambers, arXiv:1408.2508

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