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Real-time time-correlation approach for x-ray absorption and emission spectra[1] F.D. VILA, A.J. LEE, J.J. REHR, Dept. of Physics, U. of Washington, Seattle, WA 98195 — We present a real-time approach for calculations of X-ray absorption (XAS) and emission spectra (XES) from deep core-levels, based on time-correlation functions. XAS and XES have traditionally been calculated using Fermi's golden rule in frequency space, and alternatively, using real-space Green's function (RSGF) methods. Recently, however, with the advent of very high brightness pulsed x-ray sources, calculations of time-dependent response have become a focus of attention. Here we obtain the time-correlation functions by propagating the initial, dipole-excited wavefunction with a Crank-Nicolson time-evolution operator.[2] The initial state is obtained using projector augmented wave (PAW) transition matrix elements and, for XAS, the propagation is carried out in the presence of a core hole. The approach is implemented using an extension of SIESTA and can be applied both to molecular and extended systems. Illustrative examples are presented for several systems, and yield results in good agreement with RSGF and Fermi golden rule approaches using FEFF and StoBe respectively. Finally, we discuss improvements in order to include dynamic many-body effects.

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[2]Y. Takimoto *et al.*, J. Chem. Phys. **127**, 154114 (2007).

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