

Abstract Submitted
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Real-time Approach for Core-hole Dynamics in X-ray Spectra¹

ANDREW LEE, JOHN REHR, FERNANDO VILA, U of Washington — We present a real time method to calculate dynamical core hole effects in x-ray spectra using single-determinant wavefunctions to evaluate the time-correlation series. Starting with the system in the ground state, the x-ray field suddenly creates a particle-hole pair which is propagated in real-time in the presence of the dynamically screened core-hole potential. The approach is implemented in our software package RTX², a local time-correlation based program for the calculation of x-ray absorption and emission spectra. RTX uses GPAW, a grid based electronic structure code, to calculate the time-evolution operator with a Crank-Nicolson algorithm and projector augmented wave transition matrix elements. This implementation builds in full-potential electronic structure and dynamical core-hole screening, resulting in a practical and generally applicable code. Recent improvements include electron-electron interactions which had been previously neglected. By introducing the single-determinant wavefunctions, we now model intrinsic and extrinsic interactions. The method is illustrated in a number of cases, including diamond and C60.

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²A. J. Lee, F. D. Vila, and J. J. Rehr, Phys. Rev. B **86**, 115107 (2012)

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