

Abstract Submitted
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Real Time Dynamical Core-hole Effects in X-ray Spectra¹ A.J. LEE, F.D. VILA, J.J. KAS, J.J. REHR, University of Washington, Seattle — We present an extension of the real-time x-ray spectroscopy code RTX² to introduce dynamic effects due to the sudden creation of a core hole in x-ray absorption (XAS) and emission (XES) spectra. RTX is based on a local, time-correlation function approach using a real-time extension of the SIESTA code with a Crank-Nicolson time-evolution operator, and projector augmented wave (PAW) transition matrix elements. Originally RTX used a statically screened core hole, an approximation equivalent to the final state rule as in Δ SCF approaches. To introduce dynamic effects, we now start with the system in the ground state, suddenly introduce the core-hole, and then propagate the system in real time, again with the Crank-Nicolson approach. This implementation yields a generally applicable code that builds in full-potential electronic structure and dynamic core-hole screening. Illustrative examples are presented and compared with initial and final state rule approximations.

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