

Abstract Submitted  
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**Real-time TDDFT calculations of core-hole spectral functions<sup>1</sup>**

J.J. KAS, J.J. REHR, A.J. LEE, F.D. VILA, U. Washington — Core-hole response is important in a variety of x-ray spectra, including x-ray absorption, resonant and non-resonant inelastic x-ray scattering, and x-ray photo-electron spectroscopy, but has usually been treated within the adiabatic approximation. Here we explore the dynamic response of valence electrons to the sudden appearance of a deep core-hole using real time time dependent density functional theory (RT-TDDFT). The core-hole is treated as a transient time dependent potential which excites the valence electrons, as in the edge-singularity theory of Nozieres and De Dominicis. RT-TDDFT provides an efficient approach for treating response to time-dependent external fields including interactions among the valence electrons, which has recently been applied to calculations of optical and x-ray spectra.<sup>2</sup> Here we generalize this approach to explore the role of the strength and localization of the core-hole potential and its effects on the spectral function and various x-ray spectra, together with comparisons to the adiabatic approximation.

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<sup>2</sup>A. J. Lee, F. D. Vila, and J. J. Rehr, PRB **86** 115107

Joshua Kas  
U. Washington

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