

Abstract Submitted
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First-principles simulation of transient x-ray absorption spectroscopy of photo-excited molecular systems DAS PEMMARAJU, Lawrence Berkeley National Laboratory and Stanford Linear Accelerator Laboratory, KRISTINA CLOSSER, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, SIMES MOLECULAR FOUNDRY COLLABORATION COLLABORATION — We explore the utility of beyond-ground-state density functional methods such as constrained density functional theory (c-DFT) and time-dependent density functional theory (TDDFT) in the interpretation of time-resolved X-ray absorption spectroscopies investigating chemical dynamics in photo-excited molecular systems. Recent results based on a methodology that combines a state-by-state self-consistent field description such as c-DFT with a frequency domain linear-response TDDFT approach to model the core-level spectroscopy of photo-excited ring-opening dynamics in small molecular systems is discussed. Illustrative case studies involving the strong-field ionization of Selenophene and resonant UV-vis excitation of 1,3-cyclohexadiene are presented.

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