

Abstract Submitted  
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**First Principles Modeling and Interpretation of Ionization-Triggered Charge Migration in Molecules**<sup>1</sup> ADAM BRUNER, SAM HERNANDEZ, FRANCOIS MAUGER, PAUL ABANADOR, METTE GAARDE, KEN SCHAFER, KEN LOPATA, Louisiana State Univ - Baton Rouge — Modeling attosecond coherent charge migration in molecules is important for understanding initial steps of photochemistry and light harvesting processes. Ionization triggered hole migration can be difficult to characterize and interpret as the dynamics can be convoluted with excited states. Here, we introduce a real-time time-dependent density functional theory (RT-TDDFT) approach for modeling such dynamics from first principles. To isolate the specific hole dynamics from excited states, Fourier transform analysis and orbital occupations are used to provide a spatial hole representation in the frequency domain. These techniques are applied to hole transfer across a thiophene dimer as well as core-hole triggered valence motion in nitrosobenzene.

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Adam Bruner  
Louisiana State Univ - Baton Rouge

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