

Abstract Submitted  
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**Probing core-hole wavepacket dynamics in molecules using angle-resolved photoelectron spectroscopy**<sup>1</sup> SIDDHARTHA CHATTOPADHYAY, Kansas State University, LUDGER INHESTER, Center for Free-Electron Laser Science, DESY, ROBIN SANTRA, Center for Free-Electron Laser Science, DESY, Universitt Hamburg, ARTEM RUDENKO, DANIEL ROLLES, LOREN GREENMAN, Kansas State University — Attosecond dynamics have been predicted following core ionization, including charge migration and core-hole dynamics. The angular correlations in photoelectron angular distributions from the core-hole states gives direct access to probe ultrafast quantum dynamics. Attosecond x-ray pump-probe measurements, which will be available with LCLS-II, first core ionize a molecule and then probes its dynamics. In the present work, we use variational scattering calculations for the continuum states of the N<sub>2</sub> molecule. Our scheme is based on two different approximation, first using the atomic cross-section the angular correlation between two photo-electrons shows prominent oscillations with respect to the time delay between the two pulses. In the second approach, we use the electronic structure of the neutral and the ionized molecule in the Hartree-Fock approximation to obtain a more accurate description. This calculation shows that the dynamics can be observed for both single-site and two-site double-core-hole states in contrast to the atomic approach. The calculation based on the molecular potential allows us to study charge migration in complex polyatomic molecules after core-ionization.

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