Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Vibrational coherence induced by intramolecular photoelectron scattering[1] BEJAN GHOMASHI[2,4], Dept. Physics[2], University of Colorado, Boulder, NICOLAS DOUGUET[3], Dept. Physics[3], Kennesaw State University, LUCA ARGENTI[4,5], Dept. Physics[4] and CREOL[5], University of Central Florida — We study theoretically in real time, with the help of a 1D model, the photoionization of a neutral hetero-nuclear diatomic molecule from a localized core orbital. The nuclear motion is modeled with a simple harmonic oscillator, with identical parameters in both the neutral and ionized state of the molecule, within the Born-Oppenheimer approximation. Even within this elementary framework, the system exhibits strong deviations from the Frank Condon approximation, due to the recoil associated to the photoelectron emission, and to the intramolecular scattering of the photoelectron. As a consequence, the ionization of the molecule leaves behind a vibrationally excited ion. The vibrationally resolved signals in the photoelectron spectrum map holographically the intramolecular photoelectron scattering dynamics as well as the coherence of the vibrational state of the residual ion. We compute the time-dependent density matrix and Wigner distribution of the parent-ion, and show that the ion residual coherence manifests itself in an effective delay in the periodic oscillation of the excited vibrational wave packet created by the ionization event.

[1]Work supported by NSF Grants No. PHY-1912507 and DOE Grant No. DESC0020311.

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Date submitted: 31 Jan 2020 Electronic form version 1.4