

Abstract Submitted
for the DAMOP19 Meeting of
The American Physical Society

Ultrafast coupled electron-nuclear dynamics following ionization of propiolic acid ALEXANDER KULEFF, Heidelberg University — Due to the electron correlation, the removal of an electron from a molecular orbital can trigger ultrafast, pure electron dynamics [1]. The hole charge created by the ionization can migrate throughout the molecule on a few-femtoseconds timescale even at frozen nuclei [2]. The slower nuclear dynamics is expected to dephase the pure electronic coherence at a later stage and trap the migrating charge. A full-dimensional quantum calculation of the concerted electron-nuclear dynamics following the outer-valence ionization of the propiolic acid molecule will be presented, showing that the charge created upon ionization of the HOMO will oscillate between the carbon triple bond and the carbonyl oxygen for more than 10 fs before getting trapped by the nuclear motion [3]. Contrary to recently reported calculations showing an ultrafast dephasing of the charge migration by the nuclear motion, the present results suggest that longer-lived electron coherences can exist even in polyatomics.

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[2] A. I. Kuleff and L. S. Cederbaum, *J. Phys. B* **47**, 124002 (2014).

[3] V. Despré, N. V. Golubev, and A. I. Kuleff, *Phys. Rev. Lett.* **121**, 203002 (2018).

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Date submitted: 22 Jan 2019

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