Contribution ID: **13** Type: **Talk**

Coupled electron-nuclear dynmaics following ionization of propiolic acid

Thursday 15 February 2018 10:00 (20 minutes)

Due to the electron correlation, the removal of an electron from a molecular orbital can trigger ultrafast, pure electron dynamics. The created by the ionization hole charge can migrate throughout the molecule on a few-femtoseconds timescale even at frozen nuclei. The slower nuclear dynamics is expected to dephase at a later stage the pure electronic coherence and trap the 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. 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.

Primary author: KULEFF, Alexander (Heidelberg University)

Presenter: KULEFF, Alexander (Heidelberg University)

Session Classification: Attosecond 2

Track Classification: Contributed talk