Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Professor Dr. Hans Jakob Wörner
Laboratorium für Physikalische Chemie

Invitation to a Seminar on Theoretical Chemistry, Molecular Spectroscopy and Dynamics

Speaker: Dr. Oriol Vendrell
Center for Free-Electron Laser Science, DESY, Hamburg, Germany

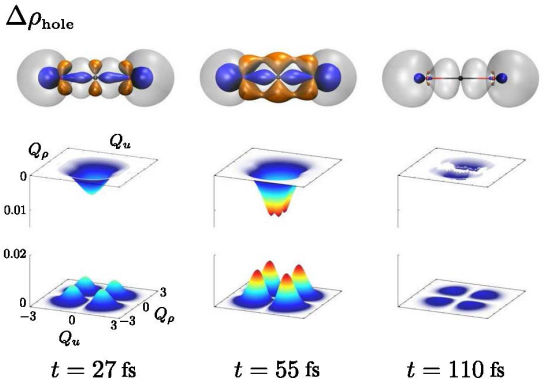
Subject: Nuclear and electronic dynamics after photo-ionization

Place: HCI J6

Date/Time: Friday, October 10, 2014, 16^{45} h

There is a fundamental interest in understanding the coupled nuclear and electronic dynamics associated to charge transfer processes in complex molecules and materials, which is often mediated by electron, electron hole or proton motion. With dramatic improvements in the techniques to generate extreme ultraviolet (XUV) femtosecond and attosecond pulses, it becomes now possible to trigger and probe these kinds of processes in real time. As an example of such fast dynamics, the response of hydrogen atoms to a newly created electron hole in a water cluster can be as fast as sub 5 fs [PRL 110, 038302 (2013)] and involve strong nuclear-electronic couplings. I will also discuss recent experiments and calculations on the creation of a coherent electron hole in CO_2^+ upon ionization by a short XUV pulses, and how non-adiabatic couplings play a decisive role in the subsequent electron hole dynamics [PRL 113, 113003 (2014)].

Figure caption: Hole density and vibronic wavepacket density of the asymmetric stretch and bending coordinates in CO_2^+. The nuclear dynamics corresponding to the bending and asymmetric stretch occurs in sync with the electron hole motion.



Guests are welcome

Frédéric Merkt, Martin Quack, Markus Reiher, Ruth Signorell, H. J. Wörner