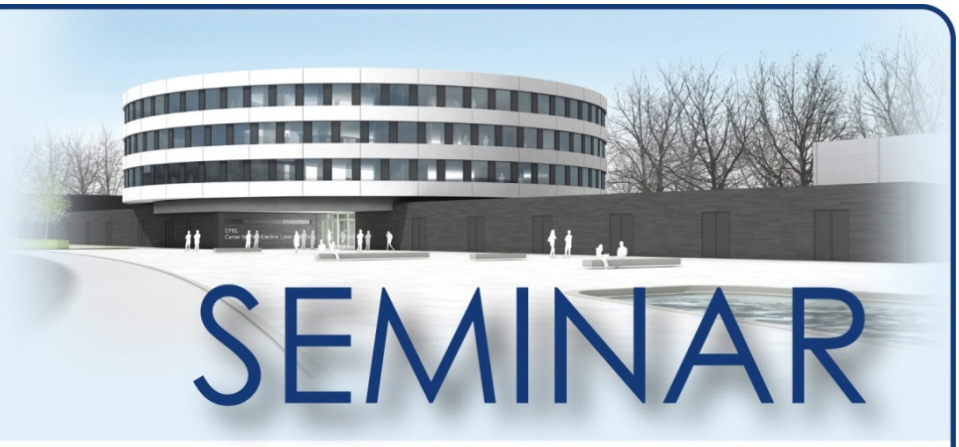
CFEL SCIENCE



SEMINAR

8th May 2024 - 2:00 p.m.

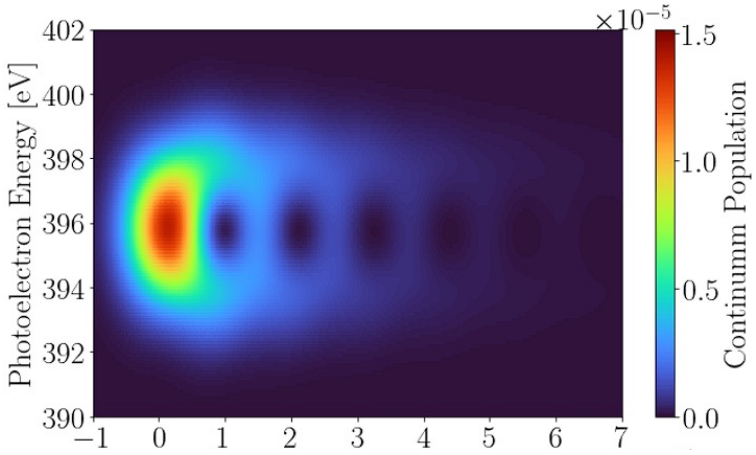
CFEL-bldg. 99, seminar room IV

Oriol Vendrell

Institute of Physical Chemistry, Universität Heidelberg, Heidelberg, Germany

Coherence and non-adiabaticity tracked with time-resolved x-rays

Under adiabatic conditions, the electrons follow the nuclei instantaneously and, in turn, the nuclei move on a single potential determined by the electronic cloud. In this regime, the electronic states are well separated compared to typical vibrational energies. However, most photo-physics and photo-chemistry take place under conditions where this approximation breaks down, with dramatic consequences for the short-time dynamics after photo-absorption, the stability of photo-excited molecules, and the underlying mechanisms of charge and energy transfer triggered by light. Ultrashort x-ray pulses appear as an ideal tool to unravel these coupled nuclear-electronic dynamics in their natural time-scales and with element specificity. In this talk, we shortly review the theoretical description of quantum molecular dynamics, the connection between non-adiabaticity and electronic coherence, and opportunities to track these dynamics using ultrafast x-rays.



[1] A. Freibert *et al.*, "Femtosecond X-Ray Absorption Spectroscopy of Pyrazine at the Nitrogen K-Edge: On the Validity of the Lorentzian Limit," *J. Phys. B* **54**, 244003 (2021).

[2] A. Freibert *et al.*, "Time-Dependent Resonant Inelastic X-ray Scattering of Pyrazine at the Nitrogen K-Edge: A Quantum Dynamics Approach," *J. Chem. Theory Comput.* **20**, 2167 (2024).

[3] E. Rodriguez-Cuenca *et al.*, "Core-hole Coherent Spectroscopy in Molecules," (under review).

Host: Robin Santra – CFEL-DESY Theory Division