CFEL SCIENCE

# SEMINAR

**12th May 2016 - 10:00 h**

CFEL – Building 99, seminar room I+II (ground floor)


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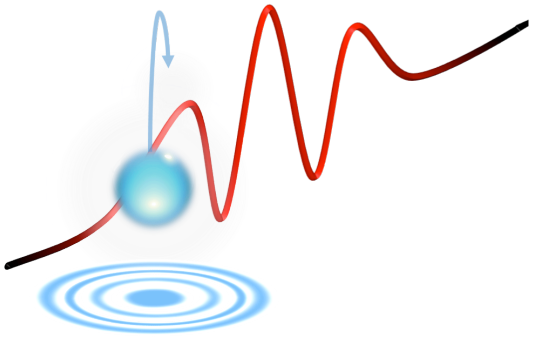
## Structure-resolved ultrafast dynamics in complex molecules by photoelectron diffraction

One of the ultimate goals of molecular physics is the possibility of manipulating the structural dynamics of molecules through external fields [1]. To this end, one first has to image the molecular structure and dynamics with an extremely high temporal resolution and atomic spatial resolution simultaneously. In this perspective, laser-induced electron diffraction (LIED) is an excellent candidate to this end [2].

In the talk I'll give an overview of my LIED experimental project and the perspectives towards the investigation of 3D-structure-resolved molecular dynamics with extremely high temporal resolution. In the first part of the talk I'll describe some basic concepts at the basis of photoelectron diffraction, underling the important implications of this technique with respect other well established diffraction methods. In particular, recent results of XUV diffraction from clusters and nanodroplets will be presented as an important example of a large-scattering-angle diffraction experiment and structure solving, in comparison with photoelectron diffraction.



The second part of the talk will concern the description of the experimental project I would like to develop, in which the time-dependent three-dimensional structure of a complex molecule could be accessed with a few-femtosecond temporal resolution. In the third part of the talk I'll analyse the theoretical concepts that are required to retrieve the dynamical molecular structure from a photoelectron diffraction pattern and, alternatively, simulate a numerical LIED experiment. In this perspective, the state of the art of quantitative rescattering theory [3] combined to Independent Atomic Model (IAM) and TD-DFT calculations applied to photoelectron diffraction will be presented [4].


[1] Y-P Chang et al, International reviews in physical chemistry **34**(4), 557-590 (2015) [2] T. Zuo et al., Chem. Phys. Lett. **259**, 313–320 (1996)
[3] Z. Chen J. Phys. B: At. Mol. Opt. Phys. 42 (2009) [4] S.-K. Son and S.-I Chu, Phys. Rev. A **80**, 011403 R (2009)


**Host: Jochen Küpper/ CFEL Molecular Physics Seminar**