Contribution ID: **82** Type: **not specified**

ultrafast time-resolved optical absorption spectroscopy studies of solvated molecules

Our group focusses on understanding photochemical reactivity in molecular systems with ultrafast x-ray and optical sources. In particular, we concentrate on smaller molecular model systems in solution as well as complex transition metal coordination compounds with relevance for e.g. solar energy or photoswitching applications, with the goal of tracking and controlling their excited state dynamics. Many of the light driven phenomena of direct relevance to molecular functionality occur on the femtosecond to picosecond time scale and involve rearrangements of electronic and nuclear structure on the Ångström length scale. This makes ultrafast x-ray methods ideally suited to advancing our understanding of these ultrafast chemical processes. Specifically, we develop and exploit ultrafast x-ray methods to track charge, spin, solvation, and coordination dynamics with atomic specificity and resolution following optical excitation. These experiments are performed at X-ray Free-Electron Laser (XFEL) and synchrotron sources worldwide. These studies are combined with complementary ultrafast optical spectroscopy experiments, simple inorganic synthesis, and simulation to identify the molecular properties that dictate excited state and photochemical processes.
In our femtosecond transient absorption spectroscopy (TAS) experiments the quality of our measured spectra depends critically on the properties and stability of our probe source, a broad-band white light continuum (WLC). For our setup we employ different WLC generation schemes using solid state conversion crystals or noble gases, and each of them produces WLC with different characteristics, including the wavelength range that is covered. In this internship we will explore the signal quality of pump-probe TAS spectra for the different WLC probes with respect to the input parameters, such as input laser intensity, gas pressure etc. The results from these studies will then i) serve as an input to select the most suitable parameters and WLC generation scheme for different research cases and ii) be used to perform such measurements on functional molecular photoswitches in order to unravel their ultrafast excited state kinetics. These will be analyzed with customized Matlab or Python codes. This is a great opportunity to get insight and intuition in modern time-resolved experiments in the field of physical chemistry, in particular with femtosecond optical lasers, and in addition different liquid sample delivery methods.
Experimental approach
The work will consist in its majority of work with the optical transient absorption setup with the amplified kHz laser system at European XFEL. The intern will investigate the influence of different WLC schemes on the quality and properties of the TAS spectra. Based on the results an appropriate WLC scheme will be selected for subsequent TAS measurements, where the intern will also be involved in studies on functional molecular photoswitching systems. To analyze the measured data he/she will perform a multi-parameter data analysis in Matlab or Python, with codes co-developed by the internship supervisor. If the timeframe of the internship coincides with a suitable synchrotron or XFEL experiment (currently we have a SACLA FEL (Japan) beamtime and a PETRA II beamtime scheduled in July 2024), the intern may also participate in these and gain practical synchrotron or XFEL experience.
Tasks of the intern
• Characterization of different white-light continuum generation schemes for the transient absorption spectroscopy setup at the laser laboratory on-site in Schenefeld; evaluation of their spectral stability and relation to the input parameters and quality of the measured TAS spectra
• Participation in TAS measurements on functional molecular photoswitches on-site in Schenefeld
• Analysis of the measured spectra using own codes/codes co-developed by the supervisor (Matlab or Python)
• Participation in a suitable synchrotron and XFEL beamtime may occur during the internship
• Documentation of the results and presentation to the group at the end of the internship
General information about the work group, the university and the region
Our work group is located on the campus of European XFEL in the Greater Hamburg Metropolian Region. European XFEL is an international research organization operating a 3.4 km long XFEL producing femtosecond flashes of X-rays with unprecedented brilliance. Three beamlines and six instruments allow international research teams to conduct experiments in the fields of physics, chemistry, biology, medicine and material science. European XFEL also hosts several (femtosecond) optical laser laboratories. The combination of ultrafast x-ray and laser sources makes the campus ideal for our research. The nearby Campus of the Deutsches Elektronen-Synchrotron (DESY) operates a VUV FEL (FLASH) and a third-generation synchrotron (PETRA III) and hosts several research institutes, e.g. from the University of Hamburg and the Max Planck Society, and offers additional exciting research and collaboration opportunities within our ongoing scientific collaborations.

Eligibility and qualification of the applicant.

• The candidate is required to study physics or chemistry or a related discipline.
• Required: basic knowledge about optics and ultrashort optical laser pulses as is taught in undergraduate physics lectures.
• Good organization and communication skills are expected.
• Required: Good English language skills.
• Desired: Programming skills in Matlab or Python.

Group

XFEL

Project Category

B1. Physics Data Analysis and Performance (software-oriented)

Special Qualifications

The candidate is required to study physics or chemistry or a related discipline. • Required: basic knowledge about optics and ultrashort optical laser pulses as is taught in undergraduate physics lectures. • Good organization and communication skills are expected. • Required: Good English language skills. • Desired: Programming skills in Matlab or Python.

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