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Understanding Temporal Landscapes of Photoinduced Structural changes in Polycyclic Aromatic Hydrocarbon (PAHs) dyads by pump-probe spectroscopy and photocrystallography

The internship will be an opportunity offered by the FS-SCS group in the photon science division of DESY. The FS-SCS group is mostly invested in investigating energy conversion and structural changes in molecules during chemical reactions, using different pump-probe techniques. The group is well known for studying the time-dependent electronic and spatial behaviors of the molecules under external stimuli such as light photons, heat, pressure, etc. in real time. We continue to pursue the elusive "molecular movie methods"in the fields related to time-resolved and ultrafast X-ray physics, which include various types of ultrafast X-ray and optical spectroscopy techniques as well as high-resolution ultrafast X-ray diffraction and scattering methodologies. Our study helps to shed light on how different processes that take place at different time scales in the event of a photo-induced chemical reaction, in solids or solutions, are correlated. The results also help us to understand how much of the structural changes are local and how much of the structural dynamics is distributed through inter-atomic or inter-molecular interactions, in the system. We also spend a lot of time researching on designing the pump-probe experiments need for investigating the temporal landscapes in the structure of complex matters during the course of a chemical or biochemical reaction.
The polycyclic aromatic hydrocarbons (PAHs) such as pyrene- or anthracene-based systems are known to form complex structures through the formation of excimers, charge transfer states, triplets, etc. upon photoexcitation. However, photoinduced reactions in the context of PAHs in molecular dyad crystals have not been studied in great details, especially, when intermolecular interactions are overwhelming. For example, the excimer formation by intermolecular non-covalent interactions is not studied much in the context of pyrene and N, N'-dimethylaniline (DMA) -containing dyads, where electron-rich DMA is connected to relatively electron-poor, pyrene. Due to its planar structure, pyrene or DMA is already known to be susceptible to π···π stacking, essential for excimer formation. The need for functionalizing pyrene comes from the idea of overcoming the excimer formation by π···π stacking. Nonetheless, several examples of excimer-induced enhanced emission (EIEE) have been reported, which encourages excimer formations to be well utilized in designing multifunctional optoelectronic materials.
In the present project, the intern will go through a series of pyrene-bridge-DMA and anthracene-bridge-DMA dyads where different kinds of bridging groups are covalently connecting the electron rich DMA to pyrene or anthracene. There are already single crystals for several molecules available. The single crystal X-ray diffraction measurements using the single crystal X-ray diffractometer available in the group would allow the intern to investigate the intermolecular interaction patterns in the crystals. He/she will be also able to process the time-resolved spectroscopic and (if time permits) some pump-probe photocrystallographic datasets collected at synchrotron facilities for some of these molecules, to process and understand the dynamics of different photoinduced reactions in different media. For the same project, the intern may also get involved in setting up crystallization for some of these molecules. The training will help him/her to understand the geometry and logistics of these experiments. How different software packages or programming codes are used to process these datasets. The student will also gain hands-on experience in steady-state optical spectroscopic and single-crystal X-ray diffraction measurements. Moreover, the student will gain important knowledge on how to combine spectroscopy and crystallography while deciphering the temporal landscapes of stimuli responsive reactions. The opportunity will provide a firsthand learning experience to an undergraduate student with a physics/chemistry or related background, to go through the cutting-edge experimental and theoretical techniques that involve our research at the FS-SCS. We believe the experience will be quite helpful for the students aspiring for a future in the field of scientific research, academia, or industry.

Group

FS-SCS

Project Category

A4. Development of experimental techniques

Special Qualifications

DESY Site

Hamburg

Primary author: BASUROY, Krishnayan (FS-SCS (Strukturdynamik Chemischer Systeme))

Presenter: BASUROY, Krishnayan (FS-SCS (Strukturdynamik Chemischer Systeme))