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# Investigation of excimer formation in purely organic molecular dyad crystals by time-resolved spectroscopy and photocrystallography

The internship will be an opportunity offered by the FS-SCS group in the photon science division of DESY to work for a limited period, on an onsite project. Interns are usually undergraduate students with physics or related background and the internship lasts for close to 6-7 weeks. Students who are invited for on-site projects are expected to work 39 hours a week and will be paid by the FS-SCS group.

Excimers, the excited state dimers are the FS-SCS group is mostly invested in investigating energy conversion and structural changes in molecules during chemical reactions, using different photon-based technologies. The group is well known for studying the time-dependent electronic and spatial behaviors of the molecules under external stimuli such as light photons, in real time. The group continues 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 what type of apparatus needs to be built and which kind of methods need to be developed for investigating the created ultrafast "time stamps"in the structure of complex matters during the course of a chemical or biochemical reaction.

The pyrene-based systems are known to form excimers upon photoexcitation. However, excimer formation by intermolecular non-covalent interactions is not studied much in the context of pyrene and 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 □···□ stacking, essential for excimer formation. The need for functionalizing pyrene comes from the idea of overcoming the excimer formation by □···□ 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 dyads where different kinds of bridging groups are covalently connecting pyrene and DMA. 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 check which of the above-mentioned molecular dyads form either homo or heteroexcimers in the crystals. He/she will be also able to process the time-resolved spectroscopic and photocrystallographic datasets collected at synchrotron facilities for some of these molecules, to process and understand the dynamics of the excimer formation process in different media. For the same project, if time permits, 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 solid-state reactions, in real-time. The opportunity will provide a first-hand 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

A2. Molecular sciences

## Special Qualifications

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