



2020 HGF – OCPC – Programme for the involvement of postdocs in bilateral collaboration projects

Title of the project:

X-ray photophysics of hydrogen-bonded molecular systems

Helmholtz Centre, division/group:

DESY, CFEL Controlled Molecule Imaging (FS-CFEL-CMI)

Project leader:

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<https://www.controlled-molecule-imaging.org>
<https://www.desy.de>

Department/Group: (at the Helmholtz centre or Institute)

Center for Free Electron Laser Science (CFEL)
Controlled Molecule Imaging Group

Programme Coordinator (Email, telephone and telefax)

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Description of the project (max. 1 page):

Properties of atoms and molecules are strongly dependent on their environment. Hydrogen bonds are of universal importance in chemistry and biochemistry and it is, therefore, of great interest to bridge the gap between single isolated molecules and molecules in solvation. In this project we plan to investigate molecular properties and the dynamics of well-defined super-molecular compound systems, i.e. hydrogen-bonded clusters, by studying their photofragmentation after atomic site-specific x-ray ionization. Our model systems include water dimers, indole-water₁, and pyrrole-water₁ clusters. The photophysics of indole and pyrrole chromophores is of the highest biological relevance, as these molecules are important building blocks of life and relevant for the understanding of the



ultrafast dynamics of larger biomolecules, such as tryptophan, vitamin B12, chlorophyll, adenine, hemoglobin, and many proteins. Our model systems have a well-defined structure, in which water is attached to the hydrogen atom which is bonded to the nitrogen atom via a single hydrogen bond. Photoionization will result in a redistribution of charges in the system. The charge redistribution processes and fragmentation channels are strongly affected by the presence of the water molecule. Observing these changes as a function of the distance between the two moieties will provide deeper insight into the role of the environment around the chromophores in biological matter. The planned experiments will be performed at modern x-ray facilities such as the Petra III synchrotron and the free electrons laser European XFEL and FLASH.

Description of existing or sought Chinese collaboration partner institute (max. half page):

Required qualification of the post-doc:

- PhD in experimental physics, physical chemistry, or a related field
- Experience with ultrashort-pulse lasers is required.
- Additional skills: Experience with large scale facilities such as synchrotrons or free electron lasers, ultra-high-vacuum equipment, and electron or ion imaging.
- Language requirement: English