



IMPRS UFAST Call for PhD applications 2020/2021



Femtosecond Soft X-ray Spectroscopy of Metallocofactors

B. van Kuiken

Title of PhD Project	Femtosecond Soft X-ray Spectroscopy of Metallocofactors
Type	Experimental Theory – with a computational component
Supervisor(s)	Dr. Benjamin E. Van Kuiken (EuXFEL) Prof. Nils Huse (UHH)
Affiliation(s):	European XFEL UHH
Number of positions:	1
Abstract:	<p>Rational design of new catalytic materials requires understanding how the underlying electronic structure guides their reactivity and photochemistry. Understanding these processes requires probes that monitor chemical dynamics on ultrafast timescales to understand bond-breaking and formation. The high-brilliance and time-resolution provided by XFEL enables new studies on dilute solution-phase systems such as molecular photocatalysts and metalloenzymes. This PhD project will focus on (1) the ultrafast soft X-ray spectroscopy (XAS and RIXS) of transition metal complexes and biomolecules, (2) the design of sample handling and delivery technologies for these systems, and (3) interpretation of spectroscopic measurements using modern quantum chemical techniques.</p> <p>Requirements:</p> <ul style="list-style-type: none">• Previous experience performing and analyzing spectroscopic measurements on molecular systems ideally involving ultrafast lasers or synchrotron/FEL radiation• Experience with a programming language (python or MATLAB) and/or computational chemistry software (Gaussian, Orca, etc.) is desirable but not required• Ability to work regularly outside usual office working hours (during beamtimes working times include nights and weekends)• Good communication skills and ability to work in an international and multi-disciplinary team with English as working language
Contact person for scientific questions about the project:	Benjamin E. Van Kuiken: benjamin.van.kuiken@xfel.eu