SFB 1078

Protonation Dynamics in Protein Function

Colloquium

Tue, **Nov. 19**, 2019

15:15 – 16:15

Charité – Universitäts-medizin Berlin (CCM – Mitte), Seminar Room 03.007

(Virchowweg 24, 14195 Berlin-Dahlem)

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Watching enzymes at work: room temperature diffraction and spectroscopy studies utilizing femtosecond X-ray pulses

The recent availability of fs X-ray pulses from XFELs makes it possible to probe the active site of various enzymes at room temperature in a time resolved manner without the problems of radiation damage. In the case of transition metals present at the active site it is also possible to conduct powerful element specific X-ray spectroscopic studies at RT using the same fs pulses. Conducting such studies, nevertheless is hindered by several technical bottlenecks. These include very limited experimental time available at the few X-ray laser sources currently operating, often very high sample consumption rates, availability of adequate reaction triggering mechanisms and challenges in data collection and processing. I will describe our various approaches to tackle these challenges, especially focusing on sample delivery, reaction triggering and data processing approaches. I will give several examples of systems where we collected X-ray diffraction and/or X-ray spectroscopic data. These include photoactive systems as well as a number of metalloenzymes. One major focus of our studies is Photosystem (PSII). PSII is a membrane intrinsic protein complex that catalyzes the light driven oxidation of water to molecular oxygen. To better understand the catalytic mechanism of PSII we are utilizing fs X-ray diffraction and X-ray emission as well as X-ray absorption spectroscopy at the Mn K- and L-edges. Recent results include first undamaged Mn L-edge spectra of PSII in two different illumination states, kinetic measurements of Mn oxidation state changes at room temperature using Mn Kb emission spectroscopy and time resolved crystallographic determination of the structure of several intermediates in the catalytic cycle of water oxidation.

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