

SFB  
1078



Protonation Dynamics  
in Protein Function

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17:00 – 18:30

Freie Universität Berlin

via WebEx

## ➤ Colloquium

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#### Capturing Reaction Intermediates of the Water Oxidation Reaction in Photosystem II

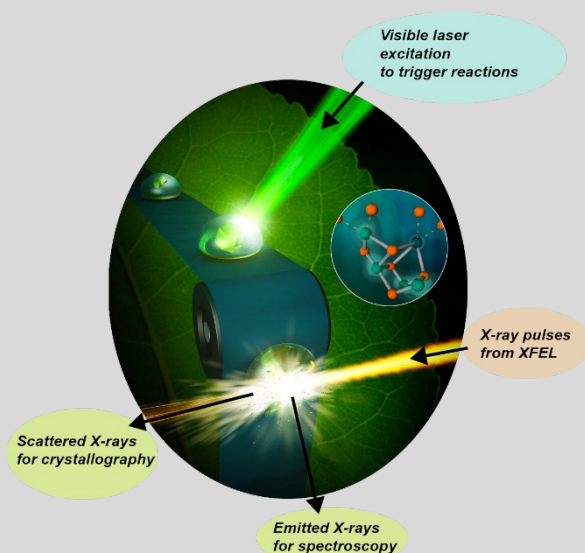
Our group is studying the mechanisms of the catalytic reactions in both natural and inorganic systems. Using various X-ray techniques as tools, we are studying how the catalysts do multielectron reactions, by following the reaction under functional conditions.

We have developed spectroscopy and diffraction techniques necessary to fully utilize the capability of the X-ray Free Electron Laser facilities (XFELs) for a wide variety of metalloenzymes, and to study their chemistry under functional conditions. One of such methods is simultaneous data collection for X-ray crystallography and X-ray spectroscopy, to look at the overall structural changes of proteins and the chemical changes at metal catalytic sites. In parallel to the detection techniques, we have developed an efficient sample delivery method that involves deposition of droplets on a conveyor belt. This 'Droplet on Tape' (DOT) method, delivers a single drop of the crystal suspension or solution sample onto a tape, which then can be transported to the X ray intersection point with a variable delay in time. In the process, the sample is photochemically or chemically activated at various time delays to capture reaction intermediates with crystallography and spectroscopy.

The presentation will cover our group's recent results of metalloenzyme research, in particular, for the study of the water oxidation reaction in natural photosynthesis, using X-ray crystallography and X-ray spectroscopy at XFEL facilities.

#### References:

- Fuller, F. D. et al.**, Nat. Methods 14, 443 (2017) DOI:10.1038/nmeth.4195.  
**Kubin, M. et al.**, Struct. Dynamics 4, 054307 (2017) DOI: 10.1063/1.4986627.  
**Kern, J. et al.**, Nature 563, 421 (2018) DOI: 10.1038/s41586-018-0681-2.  
**Ibrahim, M. et al.**, Proc. Nat. Acad. Sci. U.S.A., 117, 12624 (2020)  
DOI: 10.1073/pnas.2000529117.



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