

Interdisciplinary Instrumentation Colloquium

Front-line science builds on new ideas, but also relies on breakthrough instrumentation. Work on advanced measurement techniques and instrumentation permeates the Berkeley scientific community. In spite of disparate science objectives, many efforts face common problems and can benefit from sharing experience and expertise. The monthly Interdisciplinary Instrumentation Colloquium promotes this exchange across Berkeley Lab, UC Berkeley, Space Sciences Lab, and collaborating institutions.



Speaker: Junko Yano, Molecular Biophysics and Integrated Bioimaging Division Title: Taking Snapshots of Reaction Inermediates in Metalloenzymes and Catalysts at X-ray Free Electron Lasers

Date: March 28, 2018 Location: 50 Auditorium Time: 12:00pm -1:00pm

The development of XFELs has opened up opportunities for studying the dynamics of catalysis and biological enzymes. Intense XFEL pulses enable us to apply both X-ray diffraction and X-ray spectroscopic techniques to dilute systems or small protein crystals. By taking advantage of ultra-bright femtosecond X-ray pulses, one can also collect the data under functional conditions of temperature and pressure, in a time-resolved manner, after initiating reactions, and follow the chemical dynamics during catalytic reactions and electron transfer.

We have developed spectroscopy and diffraction techniques necessary to fully utilize the capability of the XFEL X-rays 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 also 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.

We have used the above techniques to study photochemical activation of the water oxidation reaction of the Photosystem II multi subunit protein complex, in which the Mn4CaO5 cluster catalyzes the reaction. The current status of this research and the mechanistic understanding of this metalloenzyme based on the X-ray techniques is presented.