

# X-ray Crystallography and Spectroscopy of Photosystem II Using a Femtosecond X-ray Laser



**Dr. Junko Yano**

**Senior Scientist,  
Lawrence Berkeley National Laboratory**

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The development of XFELs has opened up opportunities for studying the dynamics of biological systems beyond what is possible at synchrotron radiation (SR) sources. Intense XFEL pulses enable us to apply both x-ray diffraction and 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 chemical dynamics during catalytic reactions and electron transfer. Such an approach is particularly beneficial for biological materials and aqueous solution samples that are susceptible to x-ray radiation damage.

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 (room temperature, ambient pressure). One of such methods is simultaneous data collection for x-ray crystallography and x-ray spectroscopy, to look at overall structural changes of proteins and chemical changes at metal catalytic sites. The other method is soft x-ray absorption spectroscopy of metalloenzymes by developing a spectrometer capable of studying dilute biological systems under ambient conditions.

We have used the above techniques to study the water oxidation reaction of Photosystem II multi-subunit protein complex, in which the  $\text{Mn}_4\text{CaO}_5$  cluster catalyzes the reaction. The current status of this research and the mechanistic understanding of the water oxidation reaction based on the X-ray techniques is presented.

