

BCH 252 Seminar Series



**Dr. Junko Yano, Senior Scientist, Molecular Biophysics and Integrated Bioimaging Division
Lawrence Berkeley National Laboratory**

Seminar Title: "Making Movies of Molecules - The Application of X-ray Lasers"

Biography: Dr. Yano is currently a Senior Scientist at the Molecular Biophysics and Integrated Bioimaging Division at Lawrence Berkeley National Laboratory, USA. She is also a co-principal investigator of the Liquid Sunlight Alliance (LiSA), one of the Fuels from Sunlight Energy Innovation Hub funded by US Department of Energy. Her research areas include the water oxidation in natural photosynthesis and artificial photosynthesis, catalytic reactions in metalloenzymes, application of synchrotron X-ray radiation and X-ray free electron laser techniques to biological and inorganic systems.

Abstract provided on next page.

ZOOM Link: <https://ucr.zoom.us/j/92569273073>

Meeting ID: 925 6927 3073

Passcode: 689525

Tuesday, January 17th, 2023

12:00 p.m. - 12:50 p.m. PST

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Abstract: The metal centers in metalloenzymes and molecular catalysts are responsible for the rearrangement of atoms and electrons during complex chemical reactions, and they enable selective pathways of charge and spin transfer, bond breaking/making and the formation of new molecules. Mapping the geometric and electronic structural changes at the metal sites and its surrounding during the reactions gives a unique mechanistic insight that has been difficult to obtain to date. The development of X-ray free-electron lasers (XFELs) enables powerful new probes of such structure dynamics to advance our understanding of metalloenzymes. Using XFELs 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 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 LCLS (LINAC Coherent Light Source).

References:

Fuller, F. D. et al. Drop-on-demand sample delivery for studying biocatalysts in action at XFELs *Nat. Methods* 14, 443 (2017).

Kern, J. et al. Structures of the intermediates of Kok's photosynthetic water oxidation clock. *Nature* 563, 421 (2018).

Bergmann, U. et al. Using X-ray free-electron lasers for spectroscopy of molecular catalysts and metalloenzymes. *Nat. Rev. Phys.* 3, 264 (2021).

