

WORKSHOP # 8
 October 14, 2025
 NSLS-II Bldg 745, Room 183

**Whither Metals in Biology at NSLS-II: Spectroscopy Informed by Structural Biology /
 Bioimaging and Vice Versa**

Organizers: Erik Farquhar, Martin Fuchs, Eli Stavitski

Metals play critical roles in an array of essential biological processes, with at least one-third to one-half of all proteins thought to contain one or more metal centers. Synchrotron-based tools including macromolecular crystallography, X-ray absorption and emission spectroscopies, and X-ray fluorescence imaging have played critical roles in uncovering the structure, function, and localization of metal sites in biological systems. This workshop focuses on assessing the state of current synchrotron tools for the study of metals in biology with a two-fold goal of: a.) identifying future instrument capability needs for this community at NSLS-II as part of the NEXT-III and NSLS-IIU efforts; b.) identifying opportunities to connect spectroscopic resources with crystallographic and bio-imaging capabilities that are currently available and planned for NSLS-II.

Time (ET)	Title / Topic	Speaker (Affiliation)
Oct 13, 2025		
6:00-7:30 pm Dinner (provided) - Building 742		
8:30am	Breakfast (coffee, tea, pastries) and check-in	
9:00am	Welcome	Sean McSweeney (NSLS-II)
9:05am	Background & Objectives	Erik Farquhar (CWRU/NSLS-II)
9:20am	Ironing out the details of metalloprotein structure and function	Sarah Bowman (HWI-Buffalo) [remote speaker]
9:50am	<i>Discussion</i>	
10:00am	Expanding high-resolution XAS methods to health-relevant selenoenzymes	Katherine Rush (Auburn)
10:30am	<i>Discussion</i>	
10:40am	Break (coffee, tea, snacks) / Workshop Photo	
10:55am	Off-label Uses of DNA: Metal-mediated Base Pairs for Nanoelectronics and Nanophotonics	Simon Vecchioni (NYU)
11:25am	<i>Discussion</i>	
11:35am	Application of Nuclear Resonance Spectroscopy to Iron Containing Metalloenzymes and Biomimetic Complexes	Yisong Guo (Carnegie Mellon) [remote speaker]
12:05am	<i>Discussion</i>	
12:15pm	Lunch (provided)	
1:00pm	[Flash Talk] Fortified and starved: Polyphenol mediated metal barriers in plant immunity	Dora Farago (Brookhaven National Laboratory)
1:10pm	Spectroscopic Opportunities in Rare Earth Element Biochemistry	Joseph Cotruvo (Penn State)

1:40pm	<i>Discussion</i>	
1:50pm	Tuning the Function of Artificial Metalloenzymes by Controlling Outer-Sphere Solvent Reorganization	Saumen Chakraborty (U. Mississippi) [remote speaker]
2:20pm	<i>Discussion</i>	
2:30pm	Break (coffee, tea, snacks)	
2:45pm	Defining the Geometric and Electronic Structure of High-Valent Cobalt Complexes Using X-ray Spectroscopies	Jason Shearer (Trinity University) [remote speaker]
3:15pm	<i>Discussion</i>	
3:35pm	Extended Discussion / Next Steps	
ca. 4:15pm	Adjourn	