Homogeneous Catalysis at SSRL: From Metalloenzymes to Energy Materials

Ritimukta Sarangi[1,*]

[1]Structural Molecular Biology Group, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA-94025

*Corresponding author, email: ritis@slac.stanford.edu

Research field: X-ray Absorption Spectroscopy Applications in Homogeneous Catalysis

Abstract:
Synchrotron based X-ray absorption spectroscopy (XAS) can simultaneously yield geometric and electronic structure information on metal sites involved in catalysis, providing detailed insights into their reactivity and overall catalytic mechanism. The strength of XAS is fully realized in homogeneous catalysis applications, where the molecular systems under investigation can be synthesized in pure form and reactivity typically involves clean chemical transformations. This ability to isolate and study individual catalytic species demands rigorous quantitative analysis of the XAS data, correlation with other spectroscopic techniques and strong coupling to theoretical methods, ultimately allowing holistic investigation of each species in the catalytic mechanism. The Stanford Synchrotron Radiation Lightsource (SSRL) structural molecular biology group has been an early pioneer in biological XAS applications and building on the resulting spectroscopic insights, has spearheaded a combinatorial approach to X-ray spectroscopies by developing synergistic instrumentation, experimental and theoretical methodology and robust dissemination programs for the user community. Scientific applications highlighting the strength of various X-ray spectroscopy techniques, in solving complex problems in homogeneous catalysis will be presented with focus on multimetallic enzymatic catalysis, homogeneous electrochemical catalysis and bio-inspired chemical catalysis.