MS090.O03

Spectroscopy applications in biologically relevant systems

Ritimukta Sarangi[1]
[1]*SMB, SLAC, Stanford University, Menlo Park, United States*
E-mail: ritimukta@gmail.com

First-row transition-metal containing proteins catalyze a wide range of enzymatic processes such as oxygen transport and activation, small molecule activation and electron transfer. Understanding the geometry and electronics of resting and transient intermediate species formed during catalysis is an important step towards elucidating the catalytic mechanism. X-ray absorption spectroscopy and EXAFS are powerful spectroscopic techniques for local-geometric and electronic structure determination and can be applied to both single-crystal and solution samples. A combination of X-ray spectroscopy with density functional theory calculations can present a holistic picture of the intermediates and overall catalytic mechanism.

The above approach has been applied to a variety of metalloprotein systems, which has yielded critical insight into understanding the catalytic mechanism. In this presentation methods of application of x-ray spectroscopic techniques to metalloproteins and biomimetic systems will be presented. Metalloprotein examples will include the heterometallic enzyme Acetyl CoA synthase, which catalyzes the functionalization of CO to acetyl CoA. Model system examples will include non-heme iron complexes implicated in O2 activation catalysis.

Funding Acknowledgement.
This work was performed at the Stanford Synchrotron Radiation Lightsource, which is funded by the DOE Office of Basic Energy Sciences. The SSRL Structural Molecular Biology Program is supported by the NIH National Center for Research Resources, Biomedical Technology Program and by the DOE Office of Biological and Environmental Research.
Can, M.; Giles L. J.; Ragsdale, S. W.; Sarangi, R. Biochemistry, 2017, 56 (9), pp 1248–1260
Bang, S.; Lee, Y-M.; Cho, K-B.; Nishida, Y.; Seo, M.S.; Wong, S.; Sarangi, R.; Fuhkuzumi, S.; Nam, W. Nature Chemistry 6, 934–940 (2014)
Keywords: Spectroscopy, metalloprotein, electronic structure