

525th ASRC Seminar

Date: 13:30 ~15:00, 9 July

Location: Meeting room 103, ASRC Building

Speaker: Dr. Robert K. Szilagy

(Montana State University, USA)

Title: Multi Edge X-Ray Absorption

Spectroscopy: An Experimental Tool
Made Not Just for Theoreticians

The presentation will briefly introduce the recent development in synchrotron science that enabled the general user access to X-ray absorption beamlines. It will define the way ground state electronic structural information can be extracted from the X-ray absorption near-edge structural (XANES) analysis and highlight how atomic position coordinates can be obtained for non-crystalline samples from multi-edge extended X-ray absorption fine structure (EXAFS) analysis. The experimental and theoretical foundations of XAS will be followed by selected examples for each traditional field of chemistry. The organic example will include the S-nitrosated mercaptanes, where XAS defined the chemical bonding between the thiol functional group and the NO moiety. The bioinorganic chemistry will be catalytic Fe-S cluster of FeFe-hydrogenase, which has a remarkable [6Fe-6S] cluster. This cluster has been previously described as two sub-clusters and conveniently the electronically more complex [4Fe-4S] sub-cluster was often neglected, when considering its reactivity. XAS measurements showed that the [6Fe-6S] cluster is an electronically indivisible molecule. The organometallic application will be demonstrated for a family of chloropalladium pre-catalysts that are involved in C-C bond activation and transmetalation reactions. Spectroscopically calibrated density-functional theory will be used to fill in the missing pieces of the experimental electronic structure and to link the static structural information with chemical reactivity.

<Contact>

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