# 第359回触媒化学研究センターコロキウム

## Biological and Homogeneous Catalysis, Heterogeneous Reactivity: A combined X-ray Spectroscopic and Computational Approach

Associate Professor Robert K. Szilagyi (Montana State University, USA and University of Pannonia, Hungary)

2015年3月3日（火）10:30—12:00

（創成科学研究棟3階セミナー室D）

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The presentation will provide an overview of my broad spectrum of scientific research activities from the field of metalloenzymology, homogeneous catalysts and pre-catalysis, and recent efforts in heterogeneous reactivity. Specifically, the presentation will highlight the computational success story of defining the composition, charge, and protonation state of the MoFe-cofactor of biological nitrogen fixation; the multi-edge X-ray absorption spectroscopic treatment of Fe-S biomimetic compounds of FeFe-hydrogenase, palladium and iridium-chloride pre-catalysts; and unexpected reactivity of Fe-S surface that has been modified by molecular beam surface/scattering experiments. These topics will emphasize the importance of a holistic and comprehensive consideration of chemical synthesis, spectroscopy, and theory, which are the main pillars of my laboratory. I wish to emphasize the need for systematic research design for gaining detailed electronic and geometric structural insights by taking advantage of modern computational chemistry and particularly the information content of XANES analysis. I will conclude with a brief overview of the current focus inherited from last year's stay at the Surface and Nanostructures Laboratory of University of Pannonia in Hungary, which will be the combination of Fe-S-based redox chemistry and acid/base chemistry on exfoliated clay nanoparticles. This project is being conducted as a quantum chemical engineering design task, where a broad range of computational chemical tools are used to design and predict reactivity that are evaluated in the laboratory by chemical synthesis and spectroscopy.

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Robert K. Szilagyi received his PhD from University of Veszprém, Hungary in 1998 from Prof. Lajos Bencze, a late organometallic chemist. Immediately after graduation, he went on to work for Prof. Keiji Morokuma at Emory University on bioinorganic and organometallic chemical reactivity. This followed by more than 3 years of second postdoctoral research with Prof. Edward I. Solomon, Prof. Britt Hedman, and Prof. Keith Hodgson at Stanford University and Stanford Synchrotron Radiation Laboratory. At Stanford, he gained experience in synchrotron-based experiments (spectroscopy and scattering). In 2003, he became an Assistant Professor at the Department of Chemistry and Biochemistry, Montana State University, where he earned tenure in 2009 and became Associate Professor. In 2013, he spent 7 months at Ibaraki University and worked at the Photon Factory on a sabbatical leave from Montana. In 2014, he has received a prestigious fellowship from the Hungarian Government for the entire year of working on integrating Fe-S cluster redox chemistry and clay materials toward catalytic applications.