FACULTY OF SCIENCE
Charles University

Department of Physical and Macromolecular chemistry
www.natur.cuni.cz/chemie/fyzchem

Department of Physical and Macromolecular Chemistry
invites you for a seminar
and
Professor public lecture

Exploring Reaction Mechanisms of Metalloproteins by Correlating Theory and Experiment

Lecture hall CH 3, Faculty of Science, Hlavova 8, Praha 2

on November 3rd, 2021 at 14:00

The talk will be accessible also via Zoom: https://cuni-cz.zoom.us/j/94758328674

speaker: Doc. Mgr. Lubomír Rulíšek, CSc. DSc.

Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

Among the various essential elements in biocatalysis, metalloproteins play a specific role by catalyzing reactions that would not occur under physiological conditions. The presence of metal ions is crucial for the oxidation/reduction processes, electron transfer, spin-forbidden reactions and 'difficult reactions', such as N_2, O_2, C–H bond cleavage (or formation). These processes are intimately involved in the fundamental elements of life, e.g. respiration and photosynthesis.

Enormous efforts, both experimental and theoretical, have been exerted to understand the structure and function of metalloproteins. While experiments (e.g., X-ray crystallography, various spectroscopic techniques, electrochemistry) are crucial in the initial phases of our understanding to a particular system, theoretical calculations complement these data by providing a unique one-to-one structure-energy mapping. On an example of di- and trinuclear copper proteins (tyrosinase and multi-copper oxidases), non-heme di-iron delta9-desaturase, and dizinc glutamate carboxypeptidase II, I will demonstrate that by correlating experimental and theoretical data, the reaction mechanisms of bioinorganic systems can be fully elucidated.

Organizers: Prof. Tomáš Obšil, Prof. Jiří Čejka, Dr. Jan Přech

Department of Physical
and Macromolecular Chemistry
Faculty of Science, Charles University,
Albertov 6, Prague 2
128 44, Czech Republic

Head of Department:
Prof. RNDr. Tomáš Obšil, Ph.D.
obsil@natur.cuni.cz
T: +420 221 951 289

IČO: 00216208
DIČ: CZ00216208