

Combined Theoretical and Experimental Studies of the Reaction Intermediates in the TauD enzyme

Shengfa Ye, Carsten Krebs, Martin Bollinger, Frank Neese

High-valent iron sites play a fundamental role in bioinorganic chemistry as reaction intermediate in heme- and nonheme iron enzymes. To elucidate their geometric and electronic structure and function is therefore a key in understanding the reaction mechanisms of these enzymes. In recent years, we have – in close collaboration with our experimentally working project partners - studied a variety of mono- and dinuclear iron sites in proteins and model complexes. The lecture will stress the impact of the combination of quantum chemistry and spectroscopy for the elucidation of the structures of short lived intermediates that are not amenable to crystallographic studies.