

Instructions for PhD project proposals to the Einstein Center of Catalysis (EC²) for a PhD start in Oct. 2021

Abstract:

Small Molecule Activation Regulated by Secondary Coordination and Electrostatic Effects within Artificial Non-heme Metalloproteins

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Metalloproteins perform a wide range of chemical transformations whose functions have yet to be achieved by artificial systems. The discrepancy in reactivity can be directly linked to the inability of most unnatural systems to duplicate the precise structural control of the primary and secondary coordination spheres that are present within the active sites of proteins. This project aims at developing artificial metalloproteins, by covalently linking well characterized chemical catalysts for O₂/CO₂/H⁺ reductions into the active site of a hemoprotein HTHP. The heme free HTHP host may provide a local environment around the reactive M-O₂ and M-CO₂ intermediates that may model the secondary H-bonding interaction observed in the natural enzymes. The mechanism of generated variants will be analyzed by a combination of rapid mixing and spectrophotometry (UV/Vis, resonance Raman (RR) and EPR) as well as by following turnover in crystals by X-ray diffraction. In situ characterization of reactive intermediates may provide detailed insight into the catalytic processes leading to knowledge based catalyst improvement.