UCLA College | Physical Sciences Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR

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4:00 PM | YH 4222

Mani L. Bhaumik Collaboratory -

Dongwon Yoo Seminar & Conference Hall

Model Metalloenzymes to Catalyze the Reactions of Early Life

Abstract: Metalloenzymes catalyze the challenging chemical reactions that lie at the core of vital life processes, from carbon and nitrogen fixation to photosynthesis and respiration. Native metalloenzymes use only earth-abundant transition metals and operate under mild conditions, accessing reactivity that remains largely out of reach for synthetic systems. Given the importance of these fundamental processes in the context of energy, environment, sustainability, and human health, gaining molecular-level understanding into how metalloenzymes work is of the utmost importance. To this end, we are developing protein-based models as structural, functional, and mechanistic mimics of naturally occurring metalloenzymes. Targets to be discussed in this presentation include hydrogenase, carbon monoxide dehydrogenase (CODH), and acetyl coenzyme A synthase (ACS). These nickel-containing enzymes are implicated in chemoautotrophic origins of life and play key roles in the metabolisms of ancient bacteria and archaea. However, while these enzymes are highly functional within their cellular environment, most are costly to isolate, sensitive to external conditions, and generally poorly suited for large-scale application. Additionally, the multimetallic active sites and auxiliary cofactors obscure distinguishing spectroscopic features and render detailed analyses challenging. As a result, the molecular mechanisms of catalysis remain relatively poorly understood, thwarting efforts to build biomimetic synthetic systems that act with the efficacy of native enzymes. By combining functional studies of our model proteins with diverse spectroscopic techniques and computational investigations, we can obtain a comprehensive understanding of how the electronic and geometric structures dictate reactivity in each system. Reconstructing functional metalloenzymes “from the ground up” offers direct insight into the fundamental chemical principles driving the natural systems. Looking forward, we hope to apply these principles towards engineering effective systems for energy conversion reactions while learning about fundamental chemical transformations that may underlie the evolution of prebiotic processes into early life.

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