Special Bio-Inorganic Chemistry **Seminar**

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"Chemical and Biological Design Approaches to Controlling Protons, Electrons, and Substrates for Sustainable Catalysis"

Abstract: The reductive transformation of small molecules into value-added products represents an attractive way to store sustainable energy in chemical bonds. Achieving this efficiently and selectively requires the careful management of not only the substrate and intermediates, but also the proton and electron equivalents. Both the synthesis of small molecule catalysts and the *de novo* design of metalloproteins offer the means to control these multi-component reactions. A commonly observed strategy in biological systems to lower the barrier to reductive protonation of small molecules is concerted proton-electron transfer (CPET). However, the application of such a strategy to chemical catalysis has been lacking due to the paucity of approaches to generate CPET donors sufficiently reactive to functionalize molecules of interest ranging from N_2 to ketones. Here, I will discuss our discovery that under the protic conditions relevant to nitrogen fixation catalysis that metallocenes can serve as CPET reagents and our subsequent design of functionalized cobaltocenes suitable to electrocatalytic CPET applications. I will then finish by touching on the computational, *de novo* design of non-heme iron proteins for O_2-activation. These enzymes utilize a co-substrate to selectively generate a reactive metal-oxo intermediate that is useful for both C–H and olefin functionalization reactions. Nonetheless, such enzymes have been thus far little explored in the context of protein engineering.

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