## C. EUGENE BENNETT DEPARTMENT OF CHEMISTRY

## Understanding the Electronic Structure and Reactivity of Carbon Monoxide Dehydrogenase Model Systems for CO2 Reduction

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The fixation of CO2 to reduced carbon compounds of higher energy will have a tremendous impact on both the economy and the environment. One strategy is to use sunlight to convert CO2 and H2O into value-added products whereby energy is stored in chemical bonds and used as needed. However, existing earth-abundant materials for CO2 fixation often require large overpotentials, suffer from poisoning by the intermediates and products formed during catalysis, and have low Faradaic efficiencies due to the formation of undesired side products. Therefore, there is a critical need to design novel catalysts that will selectively reduce CO2 to fuels and chemicals using H2O as the proton source, while operating at low overpotential. Not meeting this need will limit our efforts toward finding a solution to our environmental and energy-related challenges.

Biological organisms, such as carbon monoxide dehydrogenase (CODH) enzymes, are capable of selective and efficient CO2 fixation under mild conditions. Thus, the enzymatic pathways can serve as guidelines for the rational design of bioinspired molecular electrocatalysts for CO2RR. One CODH of great importance is the Ni,Fe-carbon monoxide dehydrogenase II from Carboxydothermus hydrogenoformans (Ni,Fe-CODH) in which the active site is called the C-cluster (Fig.1). Here, we employ computational methods to understand the electronic structure and reactivity of molecular electrocatalysts that mimic essential structural features and functions of CODH for CO2 fixation. The use of homogeneous catalysts allows us to effectively tune the environment of the active site relevant to catalysis by controlling the first, secondary and outer coordination spheres, which will lead to the rational design of next-generation catalysts for artificial photosynthesis. Our research is performed in close collaboration with experimentalists.

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