



**CHEMISTRY &
BIOCHEMISTRY**

DATE **TIME** **LOCATION**
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CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES: Leveraging Nature's Design for Selective CO₂ Reduction to Value-Added Products

Abstract:

The efficient electrochemical conversion of small molecules, particularly the selective reduction of CO₂, remains a grand challenge in energy and environmental chemistry. Nature offers blueprints for addressing this challenge: Carbon Monoxide Dehydrogenase (CODH) selectively interconverts CO₂ and CO, while Acetyl-CoA Synthase (ACS) couples CO and CH₃ fragments to form a C–C bond. Inspired by these systems, my research has focused on mimicking enzymatic strategies to achieve selective multi-electron transformations of CO₂ and related substrates. In my doctoral work, I explored CODH-inspired catalysis by encapsulating cobalt phthalocyanine (CoPc) in poly-4-vinylpyridine (P4VP) polymer matrices. This polymer–catalyst composite modulates the chemical environment across primary, secondary, and outer coordination spheres, enhancing nucleophilicity at the metal center and enabling the selective reduction of CO₂ to CO and CH₃OH. Electrochemical measurements of activity and faradaic efficiency, combined with multiscale first-principles simulations, revealed critical structure–activity relationships and informed strategies for scaling from batch electrolysis to gas-fed electrolyzers.

Building on this foundation, my postdoctoral research has turned toward ACS-inspired reactivity. Using Ni-substituted azurin as an artificial metalloenzyme scaffold, I have developed bioelectrochemical platforms for C–C bond formation between CO and methyl substrates, enabling the synthesis of S-methyl thioacetate. Through spectroscopic and electrochemical characterization, we captured the accessible oxidation states of the Ni site during catalysis, providing mechanistic insights into how protein scaffolds mediate the activation of small molecules. Together, these studies highlight how enzyme-inspired design principles, coupled with multi-scale experimental and computational approaches, can advance electrocatalysis for sustainable energy and chemical synthesis.

About the Speaker:

Dr. Kevin E. Rivera Cruz is a postdoctoral researcher at the University of California, Los Angeles, in the laboratory of Professor Hannah S. Shafaat. His research uses bioelectrochemical methods and nickel-based protein models to characterize catalytic mechanisms and drive the synthesis of value-added chemical products. His expertise spans electrochemical protein film voltammetry, molecular electrocatalysis, spectroelectrochemistry, and multi-scale computational–experimental methods. His postdoctoral research is supported by the National Science Foundation Mathematical and Physical Sciences ASCEND Postdoctoral Research Fellowship and the University of California President's Postdoctoral Fellowship Program.

Dr. Rivera Cruz received his Ph.D. in Inorganic Chemistry from the University of Michigan, where Professors Charles C. L. McCrory and Paul M. Zimmerman mentored him. His doctoral research focused on modulating CO₂ reduction activity by systematically modifying the electronic structure of molecular catalysts. He has authored 10 research articles and review papers. This work was supported by the NSF Graduate Research Fellowship Program (GRFP), the National Academies of Sciences, Engineering, and Medicine, the Ford Foundation, and GEM Fellowships.



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