



THE OHIO STATE UNIVERSITY

The William G. Lowrie Department of Chemical and Biomolecular
Engineering Graduate Program Cordially invites you to attend a seminar on
Unraveling Some Mysteries in Carbon and Hydrogen Electrocatalysis

Dr. Joe Gauthier

*Assistant Professor of Chemical Engineering
Texas Tech University*

**January 9, 2024, 11:30 AM
130 Koffolt Lab, CBEC 151 W Woodruff Ave
Reception at 11:00 AM - CBEC Lobby**

Bio

Joe Gauthier is an Assistant Professor of Chemical Engineering at Texas Tech University. Dr. Gauthier graduated *summa cum laude* with his B.S. degree in Chemical Engineering at The Ohio State University in 2015 before moving to California to pursue doctoral research at Stanford University. After spending one year as a visiting student in the Physics Department at the Technical University of Denmark, he completed his PhD at Stanford in 2020. Before starting at TTU, he spent one year as a Postdoctoral Researcher at UC Berkeley and Lawrence Berkeley National Laboratory. He is the author of more than 25 peer-reviewed publications and leads a 10-person research team at TTU comprising a mix of Ph.D., M.S., and undergraduate students. At TTU, his research program focuses on heterogeneous (electro)catalysis, ultimately with the aim of solving problems related to renewable energy conversion/storage and decarbonization of the chemical industry.

Abstract

Establishing how copper facilitates the electrochemical carbon dioxide reduction reaction (CO₂RR) to products with more than one carbon atom, C₂₊, remains a critical challenge towards achieving economic viability of the process. Under typical reaction conditions, both the bulk and local pH are alkaline, with the pH near the electrode being considerably more alkaline due to poor transport of hydroxide anions at high current density. However, the difficulties associated with probing alkaline pathways using computational methods has limited the understanding of CO₂ reduction in experimentally relevant conditions. In this work, we present computed bias—dependent electrochemical activation barriers for alkaline *CO protonation to *CHO and *COH and find that while the *CHO pathway is preferred thermodynamically, the formation of *COH is more favorable kinetically. We additionally compute bias—dependent reaction energies and activation barriers for four pathways to forming the first C-C bond in the CO₂RR and find that this process is likely driven by CO dimerization. Finally, we use a rigorously benchmarked classical potential and a simple thermodynamic model of selectivity to probe the effects of surface roughness on the CO₂RR. We find that the manner of roughening (i.e., starting from copper oxide, nitride, phosphide, sulfide, copper ion sputtering, ...) does not significantly affect the distribution of available active sites relevant for CO₂RR, suggesting that the manner of roughening does not have an effect on the intrinsic selectivity and activity. We demonstrate that the extent of roughening does not have an impact on the distribution of site reactivities, indicating that experimental observation of a roughening effect is not directly a result of new catalytic sites, but rather may be due to indirect effects, e.g., mass transport of reactants and products.