In silico searches for renewable energy catalysts through chemical compound space

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This talk will provide an overview of our group’s work using both standard and atypical computational chemistry models to elucidate atomic scale reaction mechanisms. I will introduce our toolkit of in silico methods used for modeling chemical reactions and then present how they can be used to provide insight into electrocatalytic processes. I will then introduce our progress in unraveling mechanisms for energetically efficient CO₂ reduction with aromatic N-heterocycles as well as new electrocatalyst design principles obtained from high-performance computer modeling. This talk will include our current interests in quantifying how local solvation environments influence chemical reaction mechanisms as well as computational methods needed for the reliable exploration of chemical space.