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The CO2 Reduction Mechanism of Multi-Center Iron Carbonyl Catalysts as Revealed by an AB Initio Nanoreactor

By Lee-Ping Wang
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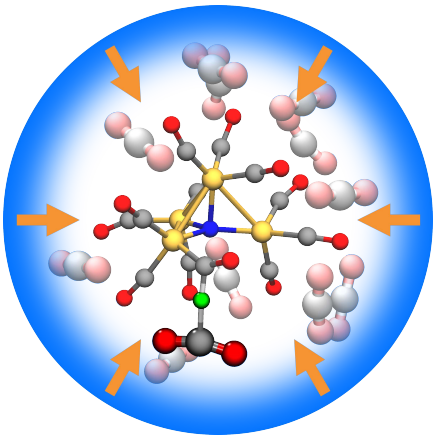
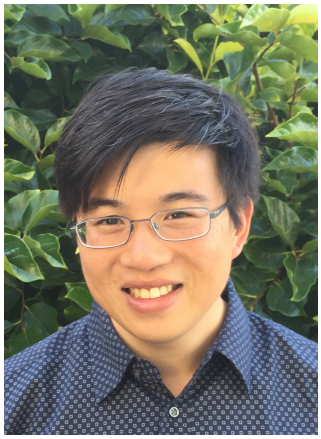
ABSTRACT



CO2 reduction is an important energy conversion pathway needed for the renewable energy economy of the future. An iron-based catalyst [Fe4N(CO)12]– has been shown to catalytically reduce CO2 to formate, providing a promising and inexpensive route toward achieving this goal. Essential questions about the mechanism of the catalyst remain unknown, such as why the catalyst is selective for CO2 reduction vs. proton reduction. In this talk, I will show some mechanistic insights provided by ab initio molecular dynamics simulations, in which a "nanoreactor" approach is employed to discover the possible reaction pathways. I will also touch on new methodologies that we have developed to facilitate the nanoreactor simulations and data analysis.

BIO:



Lee-Ping was born and raised in California, and earned his B.A. in Physics at UC Berkeley in 2006. He joined the research group of Prof. Troy Van Voorhis at MIT, where his Ph.D. research involved calculating the redox potentials and mechanisms of ruthenium and cobalt water splitting catalysts. After graduating in 2011, Lee-Ping moved to Stanford for a postdoc with Profs. Todd Martinez and Vijay Pande. During this time he developed the "nanoreactor" approach for discovering reaction mechanisms in computer simulations without relying on pre-existing hypotheses. In 2015 Lee-Ping started his new job at UC Davis, where he is now using the nanoreactor to find new mechanisms of energy conversion reactions. In a related field, Lee-Ping is also interested in molecular simulations of water and proteins, and he created the ForceBalance optimization software for improving the accuracy of molecular mechanics force fields. He has an active collaboration with Prof. LiWang to understand the fold switching pathway of the circadian clock protein, KaiB.