LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Exploring CO_2 Conversion into Commodity Chemicals with First Principles Quantum Chemistry

– John A. Keith, University of Pittsburgh

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A key component of human sustainability is the utilization of CO_2 from post-combustion processes. An intriguing avenue is the (photo-)electrochemical conversion of CO_2 into commodity chemicals such as CO, formate, and methanol. Aromatic N-heterocycle (ANH) molecules have been found to promote these reactions, but a mechanistic understanding of how this chemistry occurs is not well understood. This presentation will concentrate on our work identifying calculable pK_a and redox potential descriptors for ANH molecules to help identify which molecules at what experimental conditions would facilitate efficient (photo-)electrochemical conversions of CO_2. We will report our progress in rationalizing possible reaction mechanisms for ANH-promoted processes in light of recent experimental and computational investigations. We will also show applications of nudged-elastic band calculations in tandem with ab initio molecular dynamics simulations for unbiased analysis of CO_2 conversion mechanisms in aqueous solution.

Dr. Keith is an R. K. Mellon Faculty Fellow in Energy, a tenure-track assistant professor, at the University of Pittsburgh (Pitt) in the Department of Chemical & Petroleum Energy and affiliated with Pitt's Center for Energy. After obtaining his Ph.D. from Caltech, he was an Alexander von Humboldt postdoctoral fellow at the University of Ulm and then an Associate Research Scholar at Princeton University. He began his appointment at Pitt in September 2013. His group uses first-principles based computational chemistry to study chemical reaction mechanisms and design materials and catalysts for alternative energy conversion. Current activities address CO2 conversion, homogeneous heterobimetallic catalysis, and atomistic potential development for nanoscale simulations, all with intended applications in sustainability and renewable energy.
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