Materials Science & Engineering Seminar Series

Carnegie Mellon University
Materials Science & Engineering

presents

In Silico Searches for Efficient Renewable Energy Catalysts Through Chemical Compound Space

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ABSTRACT:

This talk will provide an overview of our group's work using both standard and atypical high-performance computational chemistry modeling to elucidate atomic scale reaction mechanisms of catalytic reactions. I will introduce our toolkit of *in silico* methods for accurately modeling solvating environments and realistic nanoscale architectures. I will then present how these methods can be used for predictive insights into chemical and material design. The talk will then summarize our progress in unraveling reaction mechanisms for 1) electrochemical CO_2 reduction with aromatic N-heterocycles and 2) CO_2 reduction on partially reduced Sn oxide materials.

BIOGRAPHY:

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 modeling to study chemical reaction mechanisms and design materials and catalysts for energy storage and conversion. Current research activities focus on atomic scale mechanisms for CO_2 conversion and tuning functional oxides via doping.

Doherty Hall 2315, 11:30AM
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