Rice University
George R. Brown School of Engineering
Department of Chemical and
Biomolecular Engineering

Presents

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Keck Hall 102

Understanding and Designing Transition Metal Catalysts

Transition metal catalysts play a critical role in the current energy landscape, enabling large scale chemical production and emissions control. Improved catalysts could increase the efficiency of these processes, and could improve the viability of clean energy technologies such as biofuels and fuel cells. However, engineering improved catalysts is impeded by two factors: understanding catalysts at the atomic scale is difficult, and the phase space for alloy catalysts is large. In this talk, I will show how theory and computation can help overcome both of these issues. Using multiscale modeling, we can gain insight into the structure and reactivity of nanostructured AgAu catalysts on various length scales. Using nonadiabatic dynamics, we can understand the role of electronic excitations in energy dissipation on surfaces. And by developing efficient, accurate, general models for adsorption, we can quickly screen surfaces for their catalytic performance.

About the Speaker

As an undergraduate, Matt Montemore majored in physics at Grinnell College. He became interested in research with energy applications, and went on to earn his PhD in mechanical engineering at the University of Colorado Boulder. His research, performed in J. Will Medlin's group in the Department of Chemical and Biological Engineering, focused on understanding and predicting adsorption on metal surfaces, with applications to catalysis and materials synthesis. For his postdoctoral research at Harvard University with Efthimios Kaxiras and Cynthia Friend, he has been using multiscale modelling, excited state dynamics, and machine learning to study the synthesis, structure, and function of nanostructured materials for catalysis.