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"FUNDAMENTAL REACTION MECHANISTIC STUDIES TOWARDS IMPROVED CATALYST DESIGN: A COMBINED THEORETICAL AND EXPERIMENTAL APPROACH"

Suyash Singh, Manos Mavrikakis

Department of Chemical and Biological Engineering, University of Wisconsin - Madison

Email: suyashsingh87@gmail.com

When:	**Monday, April 21st, 2014 3:30 pm**
Where:	**Room 265 Materials Science and Engineering**
Host:	**Prof. Izabela Szlufarska, Materials Science & Eng**

ABSTRACT:

The holy grail in heterogeneous catalysis is to understand the relationship between the surface structure and the catalytic activity and selectivity well enough to be able to design improved catalysts. To this end, we adopt a combined theoretical and experimental approach that employs first principles density functional theory (DFT) calculations, reaction kinetics experiments, and mean field microkinetic modeling, to first try and develop a complete molecular level understanding of reaction mechanisms, and subsequently design bimetallic alloy catalysts with improved performance (reactivity and selectivity) than the best monometallic catalysts. In this talk, I will discuss a case study that employs Formic Acid (HCOOH) as a model molecule to probe the reactivity of transition metals, develop trends across the periodic table, determine the optimal catalyst properties, and use this knowledge to develop a computational tool that screens for highly active and selective alloy catalysts.