

## CCST Seminar:

- › Wednesday, May 21, 2008
- › 9:30 A.M. (refreshments available at 9:15 a.m.)
- › 102/103 Colburn Laboratory



### Manos Mavrikakis

Dept. of Chemical & Biological Engineering  
University of Wisconsin-Madison

#### “The Importance of Nano-architecture in Heterogeneous Catalysis”

Catalysis is at the heart of solutions for energy and environmental problems our society is facing today. Over the last few years, periodic self-consistent Density Functional Theory (DFT-GGA) calculations have emerged as a valuable partner to experiment in explaining reactivity of transition metal surfaces. In this talk, we will attempt to demonstrate how first-principles methods can extend beyond the detailed mechanistic analysis of catalytic reactions to reach the ambitious goal of identifying promising catalysts for specific applications. Among others, we will discuss opportunities to design bimetallic and ternary alloy catalysts for highly selective hydrogen transfer reactions, and for cheaper and more active oxygen reduction (ORR) catalysts, the latter being most relevant to the cathode reaction of low temperature fuel cells. Furthermore, through a combination of theory and experiments, we will demonstrate the remarkable catalytic Preferential Oxidation (PROX) of CO in the presence of H<sub>2</sub>, as performed by core-shell bimetallic nanoparticles with precisely controlled atomic thickness for the core/shell.