

# Complexity and emergent behavior in catalytic reactions: CO oxidation on gold, biomass processing, and ammonia decomposition

## Frontiers in Catalysis Science and Engineering Seminar Series

### Presented by...

## Prof. Dionisios G. Vlachos

- Elizabeth Inez Kelley Professor
- Director of Catalysis Center for Energy Innovation
- Director of Catalytic Science and Technology
- University of Delaware



### Abstract

In this talk, complexity and emergent behavior of catalytic reactions will be presented with main focus on understanding reaction pathways, particle size and shape effects, and discovery of novel catalytic materials. Three prototype reactions will be discussed: CO oxidation on Au supported on MgO, biomass processing, and ammonia decomposition for hydrogen production. We use multiscale modeling, combining density functional theory with kinetic Monte Carlo simulations, to understand the overall activity of CO on Au particles and small clusters. We find that oxygen vacancies are critical in enabling charge transfer and thus molecular oxygen adsorption. Carbonate poisoning and catalyst restructuring are key processes in understanding activity of Au clusters. In the case of ammonia, phenomenal structure sensitivity of ammonia is found experimentally by combining EXAFS, TEM, chemisorption, and reactivity data. In particular we show that not only size but also particle shape can affect activity dramatically. Multiscale modeling is in excellent agreement with data. An approach to predicting best catalytic bimetallic materials is discussed and demonstrated experimentally. Finally, challenges and recent progress in modeling the selective conversion of biomass derivatives to chemicals are discussed.

### More info?

<http://iic.pnl.gov/>

<http://www.che.udel.edu/vlachos>

September 13, 2010

EMSL Auditorium

1:00 pm