

# Physical Chemistry Seminar

Tuesday,  
February 12, 2013

11:00 am

Room 1315  
Chemistry Building

## **A New Kind of Active Site in Heterogeneous Catalysis on Au Nanoparticles**



Professor John Yates

*Department of Chemistry  
University of Virginia*

Host: Professor JR Schmidt

Gold, usually considered to be inactive chemically, becomes very active for heterogeneous catalysis when subdivided into nanometer-sized clusters and supported on reducible oxides such as  $\text{TiO}_2$ . Such supported nanoparticles of Au feature sites at the interface between the Au and the  $\text{TiO}_2$  support which exhibit high catalytic activity for oxidation reactions. We have used transmission IR spectroscopy combined with DFT calculations to investigate the catalytic oxidation of  $\text{H}_2$ , CO and ethylene, finding that the sites responsible for activity are on the perimeter of the Au particles. Oxygen- molecule activation occurs by adsorption of an  $\text{O}_2$  molecule between a perimeter Au atom and a neighbor  $\text{Ti}^{4+}$  site, producing a  $\text{Ti}^{4+}\text{-O-O-Au}$  species which is a strong oxidizer analogous to a peroxo species. These special surface sites are called dual-catalytic sites. I will show a combination of experimental and theoretical results which all point to the unique activity of the dual-catalytic sites at the Au particle perimeter. In addition, an exotic surface species, the ketenylidene species,  $\text{Au}_2\text{C}=\text{C}=\text{O}$ , has been discovered when  $\text{C}_2\text{H}_4$  is first oxidized to acetate and then to  $\text{Au}_2\text{C}=\text{C}=\text{O}$ .

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335