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Catalysis Club of Philadelphia

Thursday, October 19, 2006

Holiday Inn Select Hotel
Naamans Road and I-95, Claymont, DE

"Experimental and computational studies of reaction pathways and size dependence in Au catalysis"

Dr. Steven Overbury

Oak Ridge National Laboratory
Chemical Sciences Division and Center for Nanophase Materials Science

&

"Redox Properties of Supported Vanadia Systems"

Parag R. Shah

University of Pennsylvania
(Student Talk, 15 minutes)

Social Hour	5:30 p.m.
Dinner	6:30 p.m.
Meeting	7:30 p.m.

Menu:

Chicken Dijonaise - *Served with a Delicate Dijon Cream*
Sliced Sirloin of Beef - *Served with a Mushroom Bordelaise Sauce*
Vegetarian Lasagna

Members	\$30.00
Walk Ins & Non-members	\$35.00
Students & Retired Members	\$15.00

For meal reservations, please notify your **company representative** or **Carl Menning** (phone: 302-893-9398, fax: 302-831-1048, e-mail: menning23@gmail.com) by **Thursday, October 12.**

Company Representatives – We would like to encourage you to make meal/meeting reservations to your company representative.

Membership – dues for the 2006-2007 season will be \$10.00 (\$5.00 for the local chapter and \$5.00 for the national club). Dues for students and post-docs will be \$6.00 (\$5.00 for local club and \$1.00 for national club). Please send your payment to Steve Harris, Lyondell Chemical Co., 3801 West Chester Pike, Newtown Square, PA 19073-2387.

Next Meeting will be held jointly with NY Catalysis Society on Thursday, November 9, 2006. The speaker will be Dr. Stu Soled of ExxonMobil.

Catalysis Club of Philadelphia

Thursday, October 19, 2006

“Experimental and computational studies of reaction pathways and size dependence in Au catalysis”

Dr. Steven Overbury

Oak Ridge National Laboratory

Chemical Sciences Division and Center for Nanophase Materials Science

Abstract

Size or structure sensitivity is well known in catalysis for many metals and for certain “demanding reactions”. Au is unusual among noble metals for its strong size dependence for the CO oxidation reaction. Au catalysts are highly sensitive to many factors relating to their synthesis and support type and so the size sensitivity is difficult to extract from comparison of many different catalysts. We have performed experiments in which Au particle size was systematically increased by a sequence of thermal treatments which are monitored *in situ* by EXAFS. Simultaneous measurements of the activity for CO oxidation permitted direct correlation between particle size and activity for a single catalyst type. Various geometric models for size sensitivity based upon Au coordination have been assessed, based on comparison with the data, and it is concluded that the rate controlling sites must be low coordinate Au sites such as corner sites or periphery sites. Microscopic evidence indicates that a change in the Au morphology from raftlike to “round” 3D particles may occur at the lowest temperatures and smallest particles size, a transformation which is accompanied by a change in activation energy. Computational studies of the effect of low coordination has also been carried out and indicate that low coordinate Au permits a flexibility in the reaction coordinate which lowers the activation barrier and makes Au more active than Pt at low temperature reactions. To better understand mechanistic aspects in CO oxidation, we have utilized a reactor capable of dynamically monitoring adsorbate species and gaseous products by FTIR and sampling mass spectrometry under transient reaction conditions. Using this transient approach, the adsorption and desorption behavior of the reactants, the competition for sites, and the the role of carbonates have been explored and the pathways for reaction have been mapped.

In a separate topic of interest to the catalysis community, a status report will be given of the Catalysis and Nano Building Block theme at ORNL’s Center for Nanophase Materials Science. A description of the facilities and the process by which researchers can become Users at the center will be discussed.

Research sponsored by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences, U.S. Department of Energy, under contract DE-AC05-00OR22725 with Oak Ridge National Laboratory, managed and operated by UT-Battelle, LLC

Speaker’s Biography



Dr. Overbury was an undergraduate at University of New Mexico with a double major in Chemistry and Mathematics. Performed graduate work at University of California under the supervision of Prof. Gabor Somorjai, and obtained PhD in December 1976. Started at Oak Ridge National Laboratory in Jan 1977 and now continues at ORNL as Distinguished Research Staff. Became group leader of the Surface Chemistry and Heterogeneous Catalysis group in 1985, and since 2003 has helped build the Catalysis and Nano Building Block theme area at the Center for Nanophase Materials Science at ORNL where he currently is the leader of this project. Currently active in the Southeastern Catalysis Society of the NACS.

“Redox Properties of Supported Vanadia Systems”

Parag R. Shah, John M. Vohs and Raymond J. Gorte
University of Pennsylvania
(Student Talk)

Abstract

Thermodynamic redox properties of vanadia (V_2O_5 , ZrV_2O_7 , and vanadia supported on zirconia, alumina, and titania) were investigated between 823 K and 923 K using Coulometric titration. For bulk V_2O_5 , there are two well-defined regimes in the oxidation isotherms, corresponding to oxidation from V^{+3} to V^{+4} and from V^{+4} to V^{+5} . The oxidation enthalpies for these two regimes are -370 kJ/gmol- O_2 and -285 kJ/gmol- O_2 , in good agreement with the literature. For zirconia-supported vanadia, the results suggest that a surface zirconium vanadate forms for vanadia loadings above one monolayer, and the isotherms for the zirconia-supported vanadia and the ZrV_2O_7 were found to be similar. For monolayer vanadia loadings on zirconia and alumina, the V^{4+} to V^{5+} transition had a heat of around -185 kJ/gmol- O_2 , compared to the value of -285 kJ/gmol- O_2 for bulk vanadia. Vanadia on titania did not show any V^{4+} to V^{5+} transition, because V^{4+} was stabilized in the solid solution with titania.

Speaker's Biography



Parag is a 3rd year PhD student at the University of Pennsylvania and is advised by Prof. Raymond J. Gorte. Parag earned his Bachelors degree in chemical engineering from the Institute of Chemical Technology, University of Bombay, and subsequently did a Masters at the University of Twente, with emphasis on Process Development and Design. Parag's current research focus is in the area of metal-oxide catalysts..

The Catalysis Club of Philadelphia: 2006-2007 Meeting Schedule

- Thursday, 9/28/06** **Prof. James Dumesic**, University of Wisconsin
2006 Catalysis Club of Philadelphia Award Lecture
“Catalytic Production of Liquid Fuels and Chemicals from Biomass-derived Oxygenated Hydrocarbons”
Rohit Vijay, University of Delaware – Student Talk (15 min)
“Discovery and Mechanistic Investigation of Cobalt Containing NSR Catalysts”
- Thursday, 10/19/06** **Dr. Steven H. Overbury**, Oak Ridge National Laboratory
“Experimental and Computational Studies of Reaction Pathways and Size Dependence in Au Catalysis”
Parag R. Shah, University of Pennsylvania – Student Talk (15 min)
“Redox Properties of Supported Vanadia Systems”
- Thursday, 11/9/06** **Dr. Stu Soled**, ExxonMobil
(Joint meeting with Catalysis Club of New York)
“Title to be announced”
- Thursday, 1/25/07** **Prof. Lanny Schmidt**, University of Minnesota
“Hydrogen from Renewable Fuels in Millisecond Reactors”
- Thursday, 2/22/07** **Prof. Galen Stucky**, University of California at Santa Barbara
“Title to be announced”
- Thursday, 3/22/07** **Dr. Andy Walker**, Johnson Matthey
“Autocatalysts: Past, Present, and Future”
- Thursday, 4/19/07** **Dr. Stacey Zones**, Chevron
“Complexities in Understanding the Synthesis and Characterization Features for High Silica Zeolites”
- Thursday, 5/17/07** **Spring Symposium**

Catalysis Club of Philadelphia Company Representatives 2006-2007

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