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Catalysis Club of Philadelphia

Thursday, September 28, 2006

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

"Catalytic Production of Liquid Fuels and Chemicals from Biomass-derived Oxygenated Hydrocarbons"

2006 Catalysis Club of Philadelphia Award Winner

Professor James A. Dumesic
Department of Chemical and Biological Engineering
University of Wisconsin – Madison

&

"Discovery and Mechanistic Investigation of Cobalt Containing NSR Catalysts"

Rohit Vijay
University of Delaware
(Student Talk, 15 minutes)

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

Menu:

Chicken Christie
Broiled Flounder - *topped with rock shrimp in a light lobster sauce*
Portabella Pasta - *grilled portabella mushroom with penne pasta tossed in a spinach cream sauce*

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, September 21.**

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 on Thursday, October 19, 2006. The speakers will be Dr. Steven H. Overbury of Oak Ridge National Laboratory.

Catalysis Club of Philadelphia

Thursday, September 28, 2006

"Catalytic Production of Liquid Fuels and Chemicals from Biomass-derived Oxygenated Hydrocarbons"

Professor J. A. Dumesic
Department of Chemical and Biological Engineering
University of Wisconsin – Madison

Abstract

We show that liquid fuels and chemicals can be produced from glycerol via a two-step process that involves the catalytic conversion of glycerol to H_2 and CO combined with the subsequent Fischer-Tropsch or methanol synthesis. Gas mixtures of H_2 and CO can be produced at high rates and selectivities from glycerol over platinum-based bi-metallic catalysts at temperatures (*e.g.*, 500-620 K) that are significantly lower compared to conventional gasification of biomass. We also show that liquid alkanes ranging from n-C_7 to C_{15} can be selectively produced by acid catalyzed dehydration of carbohydrates to produce hydroxymethylfurfural (HMF), followed by aldol-condensation over solid base catalysts to form large organic compounds. These molecules are then converted into alkanes by dehydration/hydrogenation over bi-functional catalysts containing acid and metal sites. We then show our development of a process for the selective dehydration of fructose to HMF employing a two-phase reactor system in which a reactive aqueous phase containing fructose and modifiers is contacted with an organic extracting phase (methylisobutylketone) containing additional modifiers. This system provides a cost-effective route for the synthesis of disubstituted furan derivatives that have been referred to in the literature as "sleeping giants" in the field of intermediate chemicals from renewable resources.

Speaker's Biography

James A. Dumesic earned his B.S. degree from UW-Madison and his M.S. and Ph.D. degrees from Stanford University. His Ph.D. work was conducted under the supervision of Professor Michel Boudart. Dumesic then conducted post-doctoral research as a U.S.-U.S.S.R. Exchange Fellow at the Institute of Chemical Physics in Moscow and as a NATO Postdoctoral Fellow at the Centre de Cinetique Physique et Chimique of France. Dumesic joined the Department of Chemical Engineering in 1976. He served two terms as department chair. He has been the Shoemaker Professor of Chemical Engineering, and he is currently the Steenbock Chair in the College of Engineering. Throughout his career, Dumesic has used spectroscopic, microcalorimetric, and kinetic techniques to study the surface and dynamic properties of heterogeneous catalysts. Dumesic pioneered the field of microkinetic analysis, in which diverse information from experimental and theoretical studies is combined to elucidate the essential surface chemistry that controls catalyst performance. He has developed microcalorimetric techniques to measure surface chemical bond strengths for adsorbates on metal, oxide, and acidic catalysts. He is actively involved in the use of electronic structure calculations to study the structures and reactivities of adsorbed species on metal and metal oxide surfaces. Dumesic's research group is currently studying the fundamental and applied aspects of his most recent discovery dealing with the generation of hydrogen and liquid alkanes by aqueous-phase reforming of oxygenated hydrocarbons derived from biomass.

Dumesic has received a variety of awards and honors in the field of catalysis and chemical engineering. He has been recognized with the Colburn Award and Wilhelm Award from the American Institute of Chemical Engineers, the Emmett Award from the North American Catalysis Society, and research excellent awards from the New York and Michigan catalysis societies. In 1998, he was elected to the National Academy of Engineering. He has also been recognized for his excellence in teaching at the University of Wisconsin with a Polygon Award and the 1995 Benjamin Smith Reynolds Award. In 2002, he was given the Byron Bird Award in the College of Engineering for Excellence in a Research Publication, citing his work in the microkinetics of heterogeneous catalysis. His research accomplishments were recognized in 2003 by the Herman Pines Award of the Chicago Catalysis Society. He was named one of the Top 50 Technology Leaders of 2003 by Scientific American, and he received the 2005 Cross Canada Lectureship Award of the Canadian Catalysis Society. In 2006, he received the Somorjai Award for Creative Research in Catalysis from the American Chemical Society.

"Discovery and Mechanistic Investigation of Cobalt Containing NSR Catalysts"

Rohit Vijay, Christopher M. Snively, Jochen Lauterbach
University of Delaware
(Student Talk)

Abstract

High-throughput experimentation (HTE) allows for simultaneous synthesis and screening of large arrays of different materials accelerating the discovery and optimization process. In addition, design of experiments (DOE) in combination with HTE can provide a powerful toolbox for the systematic study of vast parameter spaces encountered in the design and optimization of heterogeneous catalysts. We have applied this general approach for the study of NO_x storage and reduction (NSR) catalysts.

We have explored the effect of adding transition metals to improve the performance of platinum and barium containing NSR catalysts using the high throughput experimental set-up. Under fuel lean conditions, the addition of Mn or Fe slightly improved the NO_x storage, while the addition of Co more than doubled the NO_x storage. In addition, a noble metal free 5Co/15Ba catalyst was found to store NO_x as efficiently as a 1Pt/15Ba NSR catalyst. Characterization using XRD and TPR confirms that Co exists in different oxidation states. Transmission Electron Microscopy shows that Co and Ba are in close contact with each other and Co is uniformly distributed over the entire catalyst surface. Using in situ IR spectroscopy, we showed that Co increases the rate of nitrate formation by providing excess oxygen. Therefore, the increase in efficiency is attributed to the strong oxidizing effect of Co providing additional nitric oxide oxidation sites and contact area for NO_2 spillover to the Ba NO_x storage sites.

In order to further verify the promotional effect of Co, we have also studied the effect of adding Co to Pt/Ba or Rh/Ba based NSR catalysts as a function of cyclic operating conditions using standard statistical design of experiments. It was found that addition of Co dramatically increases the performance of both the Pt/Ba and Rh/Ba based NSR catalysts at higher lean fractions, allowing a substantial improvement in overall fuel efficiency. Preliminary conclusions from these studies also suggest that the cost of NSR catalysts can be dramatically reduced by replacing Pt with Co as the active oxidizing metal in NSR catalysts formulation. In addition, we have also optimized the catalyst composition and identified the optimum catalyst composition for Pt/Rh/Co/Ba based NSR system.

Speaker's Biography

Name: Rohit Vijay
Advisor: Prof. Jochen Lauterbach, University of Delaware
Thesis: High throughput experimentation and its applications to NOx storage and reduction (NSR) catalysts

EDUCATION

- PhD, Chemical Engineering — September 2007 (expected)
  University of Delaware, G.P.A. 3.74/4.0
- M.S., Chemical Engineering — May 2003
  Indian Institute of Technology (IIT) Madras, G.P.A. 8.8/10
- B.Tech., Chemical Engineering — May 2002
  Indian Institute of Technology (IIT) Madras, G.P.A. 8.78/10

AWARDS AND HONORS

•Awarded Garrett Reed Cantwell Graduate Scholarship for the best student of the year 2005 of the College of Engineering, University of Delaware.
•Filed for US patent on Cobalt containing NOx Storage and Reduction automotive exhaust catalysts for improving fuel efficiency of the engine and also reducing the amount of harmful gases being discharged into the atmosphere.
•The work "Cheaper Auto Exhaust Catalysts: High-throughput screening reveals promising low-cost Co-Ba catalyst" appeared in the C & E News Volume 83, Number 5, Page 9
•Won the Best Poster Award in Student poster competitions at Philadelphia Catalysis Club Meeting 2006 and at New York Catalysis Club Meeting 2006.
•Co-authored 6 papers and a book chapter titled "Design of experiments combined with high-throughput experimentation for the optimization of deNOx catalysts".
•I have also given multiple presentations at conferences like GRC, NAM, AICHE etc.