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Catalysis Club of Philadelphia

Thursday, January 17, 2008
Holiday Inn Select Hotel
Naamans Road and I-95, Claymont, DE

New Opportunities for Catalysis: Biomass to Renewable Fuels and Chemicals

Dr. Leo E. Manzer
President, Catalytic Insights LLC

&

General Trends in the Stability of Monolayer Bimetallic Surfaces

Carl Menning
University of Delaware
(Student Talk, 15 minutes)

Social Hour: 5:30 PM
Dinner: 6:30 PM
Meeting: 7:30 PM

Members: $30.00
Walk Ins & Non-members: $35.00
Student & Retired Members: $15.00

Menu
Chicken Forrestiere: *Served with Wild Mushroom Cognac Sauce*
Prime Rib: *Served with au jus*
Rigatoni a la Vodka

Meal reservations - Please notify your company representative or Carl Menning (menning@udel.edu, phone: 302-893-9398, fax: 302-831-1048) by ***Thursday, January 10***.

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

Membership - Dues for the 2007-08 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.

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New Opportunities for Catalysis: Biomass to Renewable Fuels and Chemicals

Dr. Leo E. Manzer
President, Catalytic Insights LLC
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Abstract

The rapid growth in consumption of petroleum for transportation fuels, chemicals and energy is not sustainable. Furthermore, the majority of oil reserves are in relatively unstable regions of the world. Therefore, development of technology that uses agricultural, animal, forestry and municipal solid waste as renewable feedstocks is critical to the U.S. economy and national security and therefore presents a significant opportunity for catalysis and process research.

There are many biorefinery models, but they all have the same basic issue, to provide an economically viable foundation for the production of renewable fuels. High value-added chemicals are secondary, but a key part of the refinery strategy. For gasoline, significant research programs are underway to improve ethanol fermentation, and to utilize non-food feedstocks based on lignocellulosics. Large scale biomass gasification projects are planned to produce synthesis gas which can be converted to ethanol, higher alcohols or conventional Fischer Tropsch diesel fuel. For diesel fuel, commercial plants involving transesterification of triglycerides with methanol are on the increase, while second generation technology for hydrotreating of oils and fats is approaching commercialization. Third generation biofuels based on fast pyrolysis of biomass are under development. Significant opportunities exist for the direct conversion of biomass to renewable solvents, monomers for polymers and other industrial chemicals using biological and/or thermochemical approaches. This presentation will give an overview of these emerging technologies for fuel and chemical applications.

Speaker's Biography

Leo E. Manzer is founder and President of Catalytic Insights LLC, a consulting company in the field of catalysis and process research. Dr. Manzer serves on the Scientific Advisory Board of several venture-capital funded startup companies and consults with numerous large and small companies. He was born and educated in Canada and after receiving his Ph.D. in chemistry from the University of Western Ontario, he joined the DuPont Company in Wilmington, DE. During his career at DuPont, he founded and directed the Corporate Catalysis Center and had broad responsibility for short and long term catalysis research. Dr. Manzer retired from the DuPont Company in 2005 as a DuPont Fellow. He is the author of over 90 publications and 115 US patents. He has received a number of awards, including: the 1995 ACS Earle B. Barnes Award; the 1997 Catalysis Club of Philadelphia Award; the 1997 ACS Heroes of Chemistry Award; the 1998 Cross-Canada Lecture Tour Award by the Catalysis Division of the Chemical Institute of Canada; the 2001 Eugene J. Houdry Award for Applied Catalysis from the North American Catalysis Society; and the 2003 ACS E. V. Murphree Award. He was also a member of the DuPont team recognized for the 2002 Presidential National Medal of Technology Award for his work in developing CFC Alternatives.

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General Trends in the Stability of Monolayer Bimetallic Surfaces

Carl A. Menning and Jingguang G. Chen
Department of Chemical Engineering
Center for Catalytic Science & Technology (CCST)
University of Delaware, Newark, DE 19716-3110
(Student Talk, 15 minutes)

Abstract

Bimetallic catalysts have been shown to exhibit chemical properties, such as activity and selectivity that are not simply the weighted sum of the chemical properties of the pure parent metals. One such example is the self hydrogenation of cyclohexene to cyclohexane on Pt-Ni bimetallic surfaces. While pure Pt and pure Ni show negligible activity for this reaction, the Pt-Ni bimetallic catalyst exhibits significant activity. These novel properties have been directly related to the specific configuration of the bimetallic structure in the first few layers of the bimetallic catalyst.

In this study, model monolayer bimetallic surfaces (MBS) are compared which are comprised of a host metal A with one monolayer of admetal B present in the first few atomic layers of the surface. There are three ideal MBS configurations which can be considered; the surface configuration, the mixed surface configuration, and the subsurface configuration. The surface configuration is where the 1st atomic layer of the catalyst is purely composed of the admetal B and the remaining layers are composed of the host metal A (denoted B-A-A(hkl)). The mixed surface configuration is where both host metal A and admetal B are present within the 1st layer. The subsurface configuration is where the 1st atomic layer is the host metal A, the 2nd layer contains the admetal B, and the remaining layers beyond the 2nd layer are the host metal A (denoted A-B-A(hkl)). It has been shown experimentally that it is the presence of the surface and subsurface configurations that lead to the novel chemical properties.

However, while a bimetallic catalyst may exhibit increased activity for a given reaction, it may only occur for a specific surface configuration. Therefore, an important parameter for bimetallic catalysts is the thermodynamically stability of a desired bimetallic configuration within the operating conditions of a given reaction. It will be shown that the thermodynamic stability of these configurations can be correlated with the surface d-band center. The trend for the adsorbated-induced segregation is discussed for a few common reaction environments (atomically adsorbed O, H, C, N, S, and P) on Pt-3d-Pt(111) systems (where 3d=Ni, Co, Fe, Mn, Cr, V, or Ti). In addition, the effect of switching the admetal or host metal between the 3rd, 4th, and 5th row of the periodic table is compared.

Speaker's Biography

Carl Menning received his B.S. degree in chemical engineering from the University of Minnesota-Twin Cities in 2003. Currently he is a 4th year graduate student working for Dr. Jingguang Chen in the department of Chemical Engineering at the University of Delaware. The focus of his research is on the stability of the unique subsurface configurations of platinum based bimetallics for the use as cathode electrocatalysts in proton exchange membrane fuel cells (PEMFC).