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Catalysis Club of Philadelphia

Thursday April 16, 2009

Holiday Inn Select Hotel

Naamans Road and I-95, Claymont, DE

Nanostructured Material Synthesis and Catalysis

Prof. Mayfair Kung

Northwestern University

Structure-Photocatalytic Relationships of Well-Defined TiO₂ Nanodomains

Charles A. Roberts

Lehigh University

(Student Talk, 15 minutes)

Election of new officers for the 2009-2010 season

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 - Wild

Mushroom Cognac Sauce

Prime Rib - Served with

Horseradish and light Au Jus

Vegan - Pasta Primavera

Meal reservations - Please notify your company representative or Alan Lee Stottlemeyer (alan@udel.edu, phone: 302.262.8281, fax: 302.831.1048) by **Thursday, April 9.**

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

Membership - Dues for the 2008-09 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.

Catalysis Club of Philadelphia

Thursday April 16, 2009

Holiday Inn Select Hotel

Naamans Road and I-95, Claymont, DE

Nanostructured Material Synthesis and Catalysis

Prof. Mayfair Kung

Northwestern University

Abstract

Although nano-size noble metal particles have occupied a central place in heterogeneous catalysis long before the recognition of nanotechnology, recent advances in the latter have inspired efforts to exert more precise control of both the nuclearity and the environment of the active sites of heterogeneous catalysts. In this presentation, I will discuss two types of nanocatalysts we have been investigating: nano-size zeolites and organofunctional siloxane.

ZSM-5 found wide applications as catalysts and supports. The crystal sizes of conventional ZSM-5 are often micron in dimension. For sequential reaction, where an intermediate product is desired, it can be advantageous to use nano-size zeolites. The synthesis of nano ZSM-5 with targeted morphology will be discussed.

Siloxane polymers with functional groups at predestined positions along the chain can be used to generate interesting catalytic materials. The functional groups can be used to position and stabilize metal active sites during catalyst synthesis. They can also function as the active center or affect the environment around the active center during catalytic reactions. Examples to illustrate the various uses of the organofunctional siloxane to generate catalysts of controlled nanostructures will be described.

Speaker's Bio

Mayfair Kung received her BS degree from University of Wisconsin (Madison) and her Ph. D. degree from Northwestern University. She has been involved in different aspects of heterogeneous catalysis such as selective alkane oxidation, NO_x reduction, Au catalysis, and synthesis of biomimetic catalysts. Currently, she is on the editorial board of Applied Catalysis A and Gold Bulletin.



Catalysis Club of Philadelphia

Structure-Photocatalytic Relationships of Well-Defined TiO₂ Nanodomains

Charles A. Roberts¹, Alexander A. Poretzky², Somphonh Peter Phivilay¹,
and Israel E. Wachs¹

(1) Chemical Engineering, Lehigh University

(2) Oak Ridge National Laboratory

The goal of this study was to examine the photocatalysis of well-defined TiO₂ nanodomains supported on SiO₂ and to determine their structure-photocatalytic relationships. Understanding how catalytic structure relates to photocatalytic properties (photoluminescence, electron excitation, intermediate and product formation) in these catalysts of known structure will lead to more rapid development in the discovery of improved photocatalysts for specific reactions. Thus, 1-60% TiO₂/SiO₂ catalysts were synthesized by incipient wetness impregnation of Ti-isopropoxide into the SiO₂ support (Cab-O-Sil), with drying followed by calcination at 500 °C. The molecular and electronic structures of the TiO₂ nanodomains were determined with *in-situ* Raman and UV-vis spectroscopy. The nature of the TiO₂ nanodomain was found to change in the following manner as a function of the titania loading: isolated site (1% TiO₂/SiO₂) < polymeric chain (12% TiO₂/SiO₂) < 2D sheets (20-40% TiO₂/SiO₂) < 3D nanoclusters (60% TiO₂/SiO₂). Studies were conducted using *in-situ* photoluminescence (PL) spectroscopy to determine if the type of TiO₂ nanodomain present in the sample affects the emission spectrum. Samples were dehydrated under flowing 10% O₂ at 400 °C in order to avoid the quenching effect of water on PL emission. Spectra were collected on a Jobin-Yvon Fluorolog system which also allowed collection of PL maps. Studies were also conducted *in-situ* using a 76 MHz pulsed tunable laser, tuned to 400 nm excitation, and a gated Picostar detector with time resolution in picoseconds. The same dehydration procedure was used and the lifetime of excited states of the various nano-domain containing samples was determined by changing the delay time of the detector. Production of H₂ was monitored by gas chromatography for the water splitting reaction in a UV irradiated batch reactor at room temperature.

The results show several main trends. The PL spectra show that as the percent loading of titania increases, the peak emission occurs at higher wavelength excitation, meaning those samples are more easily excited with lower energy irradiation. However, the excitation lifetime measurements indicate that the lower percent loading samples (those containing isolated TiO₂ sites) have slower decay rates, meaning there is a greater opportunity for reactions to occur. This finding offers an explanation for the observed higher production of H₂ during water splitting by the lower titania loading catalysts when normalized by exposed Ti site.

Speaker's Bio

Charles A. Roberts received his B.S. degree in Chemical Engineering from University of Notre Dame. During his undergraduate studies, he was also active in NCAA Athletics and was the Big East Champion in Hammer Throw as well as the Track and Field Team Captain in 2005. He is currently a Ph.D. student in the group of Prof. Israel Wachs at Lehigh University studying structure-photocatalytic relationships of TiO₂ catalysts. He is also the President of the Lehigh Chemical Engineering Graduate Association.

Catalysis Club of Philadelphia

Nominations are open for the 2009 Catalysis Club of Philadelphia Award

Each year the Catalysis Club of Philadelphia recognizes a person, preferably from the Philadelphia area, who has made an outstanding contribution to the advancement of catalysis. Such advancement can be scientific, technological, or in organization leadership. The award goes to an individual; no split Award to two or more persons will be given. The Award consists of a plaque and a \$1000 cash prize.

The entire nomination package, including a resume and recommendation letters, should not exceed 10 pages. The deadline for the receipt of nominations is **April 10, 2009**. Receipt of nominations will be acknowledged by email. Prior nomination packages sent in 2006 or later will automatically be considered for the 2009 Award.

Nomination letters along with supporting materials should be emailed in a single PDF document to:

Edrick Morales,
LyondellBasell Industries
3801 West Chester Pike
Newtown Square, PA 19073
edrick.morales@lyondellbasell.com
FAX: 610-359-2434
Phone: 610-359-2500

2009 Spring Symposium

The Catalysis Club of Philadelphia 2009 Spring Symposium will be held on Thursday, May 21 at the John M. Clayton Hall, University of Delaware. Invited speakers are:

Robert Schlögl, Fritz Haber Institute - Max Planck Society
Allen Burton, Chevron
Stu Soled, Exxon-Mobil Research
Chris Keily, Lehigh University
Mike Ward, New York University
Suljo Linic, University of Michigan

Program and registration information will be forthcoming.