The CATALYSIS SOCIETY of Metropolitan New York
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Chairman
SIMON PODKOLZIN
(201) 216-8074
(201) 482-5424 (fax)
Simon.Podkolzin@Stevens.edu

Secretary
XIAOMING WANG
(732) 205-6080
(732) 205-5300 (fax)
xiaoming.wang@BASF.com

Treasurer
JOHN BRODY
(908) 730-2932
(262) 313-4051 (FAX)
John.f.brody@exxonmobil.com

Wednesday, February 20, 2013
Somerset-Bridgewater Hotel, Somerset, New Jersey
(Formerly Crowne Plaza Hotel)

George B. Fitzgerald
Advisory Scientist, Accelrys, Inc., San Diego, California

Discovery of catalytic materials for automotive applications using a combined approach of informatics, modeling, and experiment

Increasing regulatory environmental requirements and consumer trends are forcing corporations to develop environmentally friendly alternatives to the status quo, and the automobile industry stands out as a highly visible example because of tailpipe emissions. Improved formulations for catalytic converters alleviate pollutants in a number of ways. Foremost, of course, they reduce CO, NOx, and hydrocarbon emissions. In the long term, however, the internal combustion engine may be replaced with 'zero emission' technologies, such as fuel cells, which will require an entirely different set of catalysts.

The number of materials that must be considered during catalyst discovery increases combinatorially with evaluation of multiple compositions and processing steps and usually reaches millions. Methods are needed that allow researchers to focus their efforts in the most promising areas. This presentation will examine how informatics and modeling are being combined with experiment to reduce the time and cost required to discover new optimum materials.

Two commercial case studies will be presented. The first is the development of materials for selective catalytic reduction to decrease NOx emissions using hydrocarbons as the reducing agent. The use of a data management system helped to increase throughput by 100-fold. The second case looks at reducing the Pt content of catalysts for the oxygen reduction reaction in fuel cells through doping with transition metals.

Qianying Guo
2012 Symposium Poster Winner
Lehigh University

Template-induced Structuring and Tunable Polymorphism of Three-dimensionally Ordered Mesoporous (3DOm) Titania Materials

The hydrothermal instability of conventional catalyst supports, therefore, demands the development of next generation materials for high-selectivity catalytic conversions in

the biofinery (e.g., dehydration/oxidation chemistries, isomerizations). Specifically, hydrothermally stable heterogeneous catalysts bearing three-dimensionally ordered mesoporous (3DOm) and hierarchical (i.e., macro-meso-microporous) pore structures are sought in order to accommodate diffusion of bulky sugar molecules and their derivatives. The enhanced hydrothermal stability and reducible structure of titania establishes its promise as a robust substrate for liquid phase biofuel catalysis. A sacrificial nanotemplating strategy involving the infiltration of colloidal crystals composed of size-tunable (ca. 10 nm and larger) silica nanoparticles with titania precursor solutions followed by confined hydrolysis therein enables the fabrication of three-dimensionally ordered mesoporous (3DOm) titania structures with controlled pore body size in the range of nanometers to tens of nanometers. The hard silica template enables calcination-induced improvement in titania crystallinity, with the templated pores robust to collapse upon template removal. This approach results in 3DOm titania materials with attractive textural properties, including surface areas (ca. 289 m^2/g) and pore volumes that are up to four times and more than an order of magnitude larger, respectively, then commercially available titania. Fundamental insight into titania polymorphism (i.e., rutile, anatase, or fraction thereof) has been elucidated as it relates to its sensitivity to the degree of titania confinement imparted by the template as well as the template surface chemistry. Specifically, increasing confinement helps to stabilize the active anatase polymorph, while tuning the degree of surface hydroxylation of the template enables fine control over fractional polymorphism, the latter having potential implications on inherent reactivity. Functionalization of these materials with both organic (sulfonic acid groups) and inorganic (Pt) moieties has been studied for the purpose of creating multifunctional dehydration-oxidation catalysts for processing of sugars. In the case of Pt functionalization, template transfer techniques are under investigation as a means for realizing uniformly distributed functionality and possible partial embedment within the 3DOm titania structures for enhancing catalyst stability.

Dinner is a buffet, and includes		Members	**$40**
a choice of beef, chicken or fish		Non-members	**$50**
Social Hour (Cash Bar)	6:00 PM	Students	**$25** (***Student Members = $10***)
Dinner	7:00 PM	Retired/Post-Doc/ Unemp.	**$40** (***Members = $30***)
Presentation	7:45 PM	Annual Dues	**$35 (Student/Retired = $15)**

Deadline for dinner reservations is **2:00 p.m. Friday, February 15, 2013**

Email Xiaoming Wang (xiaoming.wang@basf.com) for reservations. With the exception of extreme circumstances, anyone not canceling reservations by the above deadline will be billed for dinner regardless of attendance.
