

Chairman-Elect
Lucas Dorazio

Past Chairman
Marco Castaldi

Catalysis Society Representative
Israel Wachs

Webmaster
Robert McGuire

Directors
David Harris
Partha Nandi
John Byrne

The CATALYSIS SOCIETY of Metropolitan New York
www.nycsweb.org

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, October 10, 2012

Somerset-Bridgewater Hotel, Somerset, New Jersey
(Formerly Crowne Plaza Hotel)

Peter C. Stair

Professor of Chemistry, Department of Chemistry, Northwestern University
Northwestern University Center for Catalysis and Surface Science
Institute for Catalysis in Energy Processes
Institute for Atom-efficient Chemical Transformations

Senior Scientist, Chemical Sciences and Engineering Division, Argonne
National Laboratory

Oxide, Metal, and Porous Catalytic Materials by Atomic Layer Deposition

Atomic Layer Deposition (ALD) has enormous potential for the synthesis of advanced heterogeneous catalysts with control of composition and structure at the atomic scale. The ability of ALD to produce conformal oxide coatings on porous, high-surface area materials can provide completely new types of catalyst supports. At the same time ALD can achieve highly uniform catalytically active metal and oxide phases with (sub-) nanometer dimensions.

In our laboratory ALD has been used to synthesize oxide supports, catalytic oxide overlayers, metal nanoparticles, and new porous structures. These materials have been characterized by SEM, XRF, ICP, UV-Vis absorption spectroscopy, Raman spectroscopy and evaluated for catalysis of oxidative and non-oxidative alkane dehydrogenation, selective photo-oxidation, and combustion.

We have focused on the synthesis of supported metal nanoparticles and developed a procedure in which the metal and support materials are grown sequentially in each ALD cycle. This method makes possible the synthesis exceptionally small particles, ca. 0.5 nm. Using additional ALD support layers at the conclusion of the growth, a process we call overcoating, the metal particles can be stabilized against sintering and leaching while still remaining active at high temperatures and reaction conditions. The catalysts are also resistant to deactivation by coke formation. These phenomena are due to the anchoring

of step and edge atom sites while leaving facet sites open for catalysis. Through proper annealing procedures the overcoating oxide develops porosity, thus ALD becomes a method for introducing and controlling pore structures.

Tao Chen

2012 Spring Symposium Poster Winner

Stevens Institute of Technology

Spectroscopic and computational study of BPE adsorption on Ag/SiO₂ as a function of silver oxidation and adsorbate coverage

Adsorption of a commonly used spectroscopic probe molecule BPE, trans-1,2-bis(4-pyridyl)ethylene, which consists of two pyridine rings joined by a CH=CH link, was studied on monodispersed Ag nanoparticles as a function of the adsorbate surface coverage and the extent of Ag oxidation. Monodispersed Ag nanoparticles with a diameter of ~50 nm supported on silica were synthesized using a colloidal solution. The extent of Ag oxidation was varied with a time-controlled exposure to ozone and monitored with X-ray photoelectron spectroscopic (XPS) measurements.

Surface-enhanced Raman spectra (SERS) of adsorbed BPE exhibit two prominent peaks at 1590 and 1620 cm⁻¹, which are assigned, respectively, to the pyridyl ring breathing and bridging C=C stretch based on DFT calculations. The relative intensity of these two peaks was found to change with the BPE surface coverage and also with the extent of Ag oxidation. The observed changes in Raman peak intensities are attributed to differences in BPE adsorption modes. DFT calculations suggest that BPE can adsorb in two configurations: vertical and horizontal. Although both adsorption modes are energetically similar at low coverage on metallic Ag, the vertical configuration becomes more preferable with increasing coverage due to lateral interactions. The opposite effect is predicted based on DFT calculations for the increase in the extent of Ag oxidation due to the greater stability of the horizontal BPE on oxidized Ag surfaces.

The closely integrated experimental-theoretical study for the first time identified at the molecular level the adsorption modes and energetics of BPE on silver surfaces and the effects of the adsorbate coverage and the extent of Ag oxidation.

Dinner is a buffet, and includes a choice of beef, chicken or fish		Members	\$40
		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, October 5, 2012

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.

2012-2013 Officers: **Simon Podkolzin** (Chair), **Lucas Dorazio** (Chair-Elect), **Marco Castaldi** (Past Chair), **Israel Wachs** (Catalysis Society Rep), **Xiaoming Wang** (Secretary), **John Brody** (Treasurer), **Robert McGuire** (Webmaster), **David Harris**, **Partha Nandi**, **John Byrne** (Directors)