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Catalysis Club of Philadelphia

Thursday March 21st, 2013

DoubleTree Hotel
4727 Concord Pike Wilmington, DE 19803

**Sulfur-Resistant Pd-Alloy Membranes
for H₂ Purification**

James B. Miller

*Department of Chemical Engineering,
Carnegie Mellon University*

**Nature of Catalytic Active Surface Sites on
Semiconductor Photocatalysts for Splitting of
Water**

Somphonh Peter Phivilay

*Operando Molecular Spectroscopy & Catalysis Laboratory,
Department of Chemical Engineering, Lehigh University.*

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

Members: \$35.00
Walk Ins & Non-members: \$40.00
Student & Retired Members: \$20.00

Menu

- **Soy Marinated Szechuan Chicken** with Sliced Pineapple topped with a Sesame Teriyaki Glaze
- **Florentine Cod Filet** topped with Sauteed Spinach and Creamy Olive Sauce
- **Hand Rolled Vegetable Lasagna** stuffed with freshly Grilled Vegetables, Ricotta & Mozzarella Cheeses

Meal reservations - Please notify your company representative or Jacob Weiner (jlweiner@udel.edu, phone: 302.831.2213) by **Thursday March 14th**.

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

Membership - Dues for the 2012-13 season will be \$25.00 (\$5.00 for the local chapter and \$20.00 for the national club). Dues for students, post-docs and retirees will be \$10.00 (\$5.00 for local club and \$5.00 for national club).

Sulfur-Resistant Pd-Alloy Membranes for H₂ Purification

James B. Miller

Department of Chemical Engineering, Carnegie Mellon University

Abstract.

Separation of hydrogen from mixed gas streams is a key unit operation in the generation of carbon-neutral fuels and electricity from fossil- and bio-derived feedstocks. Dense Pd membranes have received significant attention for the separation application in advanced gasification processes. Pd's near-perfect selectivity reflects its unique interactions with H₂: molecular H₂ dissociates on the catalytic Pd surface to create H-atoms, which dissolve into and diffuse through the Pd bulk, to eventually recombine on the downstream side of the membrane. In practice, Pd suffers from several limitations, including high cost, structural instability, and deactivation by minor components of the mixed gas, most notably H₂S. Alloying with minor components, such as Cu, can be an effective strategy for improving membrane performance.

In collaboration with scientists at the National Energy Technology Laboratory, we have combined membrane performance testing, computational modeling, and H₂ dissociation activity characterization to provide fundamental understanding of the interactions of H₂ and H₂S with Pd and PdCu alloys. We have shown that H₂S influences membrane performance by two distinct mechanisms: surface deactivation, which inhibits the dissociative adsorption of H₂, and reaction with the metal to form a low-permeability sulfide scale. The mechanism that dominates depends on both alloy composition and operating conditions. Significantly, the surface of the sulfide scale is itself active for H₂ dissociation. Atomistic modeling of the dissociation process provides context for this observation, showing that while the energetic barrier for H₂ dissociation is higher on Pd₄S than on Pd, there exist reaction trajectories with relatively low barriers that can sustain the separation sequence at acceptable rates. Microkinetic analysis of H₂-D₂ exchange conducted over Pd and a series of PdCu alloys, both in the presence and absence of H₂S, confirms this finding and provides insight into the role of the Cu minor component in imparting S-tolerance to the alloy.

Finally, we have developed a high throughput capability to explore alloy properties over broad, continuous composition space, based on Composition Spread Alloy Film (CSAF) libraries of model separation alloys. CSAFs are thin (~100 nm) films with compositions that vary continuously across the surface of a compact (~1cm²) substrate. Using a unique multichannel

microreactor for spatially resolved measurement of reaction kinetics across CSAF surfaces, we have characterized the kinetics of H₂-D₂ exchange across continuous Pd_{1-x}Cu_x and Pd_{1-x-y}Cu_xAu_y composition space.

Biography.

Jim Miller is Associate Research Professor of Chemical Engineering at Carnegie Mellon University, where he studies advanced materials for energy-related applications in separations, catalysis and chemical sensing. Jim earned BS, MS and PhD degrees at Carnegie Mellon and an MS at the University of Pittsburgh. Before joining the faculty in 2006, he worked in industry as a developer of catalysts, catalytic processes and chemical sensors for over 25 years. Jim is a two-time past president of the Pittsburgh-Cleveland Catalysis Society; he recently led the Society's successful efforts to obtain tax exempt status in anticipation of NAM 2015. He is a winner of AIChE's 2010 "Shining Star" in recognition of his volunteer work in the Pittsburgh Local Section.



Nature of Catalytic Active Surface Sites on Semiconductor Photocatalysts for Splitting of Water

Somphonh Peter Phivilay

Operando Molecular Spectroscopy & Catalysis Laboratory, Department of Chemical Engineering, Lehigh University, Bethlehem, PA 18015, USA

Abstract.

One of society's great challenges for the 21st century is the development of alternative energy resources. Hydrogen is considered to be one of the potential candidates especially if it can be generated from the photocatalytic conversion of cheap abundant H₂O into clean non-carbon H₂ from solar energy resources. Development of this clean, renewable form of energy will help to address our reliance on depleted fossil fuel supplies and the environmental problems accompanying its use.

Photocatalytic splitting of waters proceeds via generation of excited electrons and holes in the semiconductor catalyst bulk lattice, the diffusion of the excitons through the semiconductor lattice to the surface, and surface reactions of the excitons with water to split H₂O to H₂ and O₂. The photocatalysis literature, however, has almost completely neglected the surface nature of photocatalysts and focused on the semiconductor catalyst bulk lattice that is only responsible for generation of the excited holes and electrons.

This presentation will examine the anatomy of the supported $(\text{Rh}_{2-y}\text{Cr}_y\text{O}_3)/(\text{Ga}_{1-x}\text{Zn}_x)(\text{N}_{1-x}\text{O}_x)$ photocatalysts that are able to split water with visible light excitation by determining the nature of the bulk lattice (mm), surface region (~1-3 nm) and outermost surface later (~0.3 nm) with unique cutting edge characterization techniques.