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Catalysis Club of Philadelphia

Thursday February 16th, 2012

DoubleTree Hotel

4727 Concord Pike Wilmington, DE 19803

**Fundamental Studies on the Water-gas Shift Reaction
on Metal/Oxide Catalysts: Active Sites and Reaction
Mechanism**

José A. Rodriguez

Chemistry Department, Brookhaven National Laboratory

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

Meal reservations - Please notify your company representative or Kevin Bakhmutsky (kbakh@seas.upenn.edu, phone: 215.898.0056, fax: 215.573.2093) by **Thursday February 9th**.

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

Membership - Dues for the 2011-12 season will be \$25.00 (\$5.00 for the local chapter and \$20.00 for the national club). Dues for students and post-docs will be \$10.00 (\$5.00 for local club and \$5.00 for national club).

Menu

Soy Marinated Szechuan Chicken
with Sliced Pineapple topped with a Sesame Teriyaki Glaze

Florentine Cod Filet topped with Sautéed Spinach and Creamy Olive Sauce

Vegetarian: Hand Rolled Vegetable Lasagna stuffed with freshly Grilled Vegetables, Ricotta & Mozzarella Cheeses

Vegan: Vegetable Phyllo Triangle on a bed of Ratatouille

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Fundamental Studies on the Water-gas Shift Reaction on Metal/Oxide

Catalysts: Active Sites and Reaction Mechanism

José A. Rodriguez

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Abstract:

The high-performance of gold-ceria, copper-ceria and gold-titania catalysts in the water-gas shift (WGS) reaction relies heavily on the direct participation of the oxide in the catalytic process. Although clean Au(111) is not catalytically active for the WGS, gold surfaces that are 20 to 30% covered by ceria or titania nanoparticles have activities comparable to those of good WGS catalysts such as Cu(110) or Cu(100) [1]. Over ceria/Au(111) and ceria/Cu(111) [1,2], water dissociates on O vacancies of the oxide nanoparticles, CO adsorbs on metal sites located nearby, and subsequent reaction steps take place at the metal-oxide interface. In the inverse CeO_x/Au(111) catalyst, the moderate chemical activity of bulk gold is coupled to that of a more reactive oxide. On the basis of this result, we decided to explore the catalytic activity of metal (M= Au, Cu, or Pt) and CeO_x nanoparticles dispersed on a TiO₂(110) surfaces [3,4]. At small coverages of ceria on titania, the CeO_x nanoparticles have an unusual coordination mode. Scanning tunneling microscopy and density-functional calculations point to the presence of Ce₂O₃ dimers [3]. These dimers are anchoring sites for metal nanoparticles. The M/CeO_x/TiO₂(110) surfaces display an extremely high catalytic activity for the WGS. In the M/CeO_x/TiO₂(110) systems, there is a strong coupling of the chemical properties of the admetal and the mixed-metal oxide. The adsorption and dissociation of water probably take place on the oxide, CO adsorbs on the admetal nanoparticles, and all subsequent reaction steps occur at the oxide-admetal interface [3,4].

References

1. S.D. Senanayake, D. Stacchiola, J. Evans, M. Estrella, L. Barrio, M. Pérez, J. Hrbek, and J.A. Rodriguez, *J. Catal.*, 271 (2010) 392.
2. J.A. Rodriguez, J. Graciani, J. Evans, J.B. Park, F. Yang, D. Stacchiola, S.D. Senanayake, S. Ma, M. Perez, P. Liu, J.F. Sanz, and J. Hrbek, *Angew. Chem. Int. Ed.*, 48 (2009) 8047.

3. J.B. Park, J. Graciani, J. Evans, D. Stacchiola, S. Ma, P. Liu, A. Nambu, J.F. Sanz, J. Hrbek, and J.A. Rodriguez, *Proceedings of the National Academy of Science (PNAS)*, 106 (2009) 4975.
4. J.B. Park, J. Graciani, J. Evans, D. Stacchiola, S.D. Senanayake, L. Barrio, P. Liu, J.F. Sanz, J. Hrbek, and J.A. Rodriguez, *J. Am. Chem. Soc.*, 132 (2010) 356.

Speaker Bio:

José A. Rodriguez was born in Caracas, Venezuela. He did his undergraduate education at Simon Bolivar University, receiving BS degrees in Chemistry and Chemical Engineering. After getting a MS in Theoretical Chemistry at Simon Bolivar University, he moved to the United States to get a PhD in Physical Chemistry at Indiana University, Bloomington. Currently, he is a Senior Scientist at Brookhaven National Laboratory and an Adjunct Professor at the Chemistry Department of SUNY Stony Brook. He has co-authored more than 300 articles in the areas of surface science and catalysis. His group is doing research in desulfurization processes, the synthesis of C₁-C₄ alcohols from CO/CO₂ hydrogenation, and the production of hydrogen through the water-gas shift, the steam reforming of alcohols and the photocatalytic splitting of water.

