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Wednesday, October 16, 2013
Somerset-Bridgewater Hotel, Somerset, New Jersey
(Formerly Crowne Plaza Hotel)

Jingguang Chen
Thayer Lindsley Professor of Chemical Engineering,
Columbia University, Yew York, NY 10027, USA
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Design of Catalysts and Electrocatalysts for Energy Applications

In the current talk we will use two examples to demonstrate the importance of using surface science studies to identify catalysts and electrocatalysts. Our research approaches involve parallel efforts in density functional theory (DFT) calculations, surface science experiments on model systems, and synthesis and evaluation of supported catalysts under thermochemical or electrochemical conditions. We will first use water electrolysis to demonstrate the feasibility of using monolayer Pt on tungsten carbide (WC) to achieve the same activity as bulk Pt. We will present DFT calculations of similar electronic and chemical properties between monolayer Pt/WC and Pt, synthesis and characterization of monolayer Pt/WC films, and electrochemical evaluation of the activity and stability of Pt/WC for water electrolysis. Comparing to the leading Pt electrocatalyst, the monolayer Pt/WC represents a reduction by a factor of ten in Pt loading [1,2].

We will then use the conversion of biomass-derived oxygenates to illustrate the advantages of using bimetallic catalysts. Bimetallic catalysts often show unique activity and selectivity over their parent metals due to the electronic modification and strain effect [3,4]. We will present our results on the characterization of Ni/Pt bimetallic surfaces and catalysts under in-situ reaction conditions, further highlighting the importance of using the combined approaches of DFT calculations, surface science experiments, and reactor evaluations [5,6].

[1] D.V. Esposito, S.T. Hunt, K.D. Dobson, B.E. McCandless, R.W. Birkmire and J.G. Chen, "Low-Cost Hydrogen Evolution Catalysts Based on Monolayer Platinum on Tungsten Monocarbide Substrates", *Angewandte Chemie International Edition*, 49 (2010) 9859-9862.

[2] D.V. Esposito, S.T. Hunt, Y.C. Kimmel and J.G. Chen, "A New Class of Electrocatalysts for Hydrogen

- Production from Water Electrolysis: Metal Monolayers Supported on Low-Cost Transition Metal Carbides”, *Journal of the American Chemical Society*, 134 (2012) 3025-3033.
- [3] W. Yu, M.D. Porosoff and J.G. Chen, “Pt-based Bimetallic Catalysis: From Model Surfaces to Supported Catalysts”, *Chemical Reviews*, 112 (2012) 5780-5817.
- [4] D.A. Hansgen, D.G. Vlachos and J.G. Chen, “Using First Principles to Predict Bimetallic Catalysts for the Ammonia Decomposition Reaction”, *Nature Chemistry*, 2 (2010) 484-489.
- [5] M. Saliccioli, W. Yu, M.A. Barteau, J.G. Chen, D.G. Vlachos, “Differentiation of O-H and C-H Bond Scission Mechanisms of Ethylene Glycol on Pt and Ni/Pt Using Theory and Isotopic Labeling Experiments”, *Journal of the American Chemical Society*, 133 (2011) 7996-8004.
- [6] W. Yu, M.A. Barteau and J.G. Chen, “Glycolaldehyde as a Probe Molecule for Biomass-derivatives: Reaction of C-OH and C=O Functional Groups on Monolayer Ni Surfaces”, *Journal of the American Chemical Society*, 133 (2011) 20528-20535.

Dinner is a buffet, and includes <u>a choice of beef, chicken or fish</u>		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 11, 2013

Email Zhong He (zhe@primusge.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.

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