Catalysis Club of Philadelphia

Thursday April 18th, 2013
DoubleTree Hotel
4727 Concord Pike Wilmington, DE 19803

In Situ Spectroscopic Studies of Metal Oxide Electrodes During Water Oxidation

John Kitchin

Department of Chemical Engineering,
Carnegie Mellon 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

- Roasted Prime Rib served with Whipped Potatoes, Bean Medley and a classic Demi Glaze;
- Chicken Mozzarella Sauteed Chicken Smothered with Provolone Cheese, Wild Mushrooms and Sweet Marsala Brown Sauce;
- Vegetable Wellington, Portobello mushrooms, zucchini, summer squash, spinach, roasted red pepper, Broccoli, fontina and mozzerella cheese combined in a light white wine sauce.

Meal reservations - Please notify your company representative or Jacob Weiner (jlweiner@udel.edu, phone: 302.831.2213) by ***Thursday April 11th***.

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).

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Abstract.
Electrochemical water splitting may be in integral part of future energy storage strategies by enabling energy storage in chemical bonds. One of the primary sources of inefficiency in the water splitting reaction is the oxygen evolution reaction, which has high reaction barriers that require additional applied electric potential to drive the reactions at practical rates. The most active electrode materials in acid electrolytes include ruthenium and iridium oxides, which are expensive but necessary for stability. In alkaline environments, many base metal oxides become stable, although they are still less active than Ru and Ir oxides. It has been known that small amounts of Fe can promote the electrochemical activity of nickel oxides, making it almost as active as cobalt oxide. We have investigated the mechanisms behind the promotion using in situ Raman and synchrotron spectroscopies as well as ex situ characterization techniques. Interestingly, we found the electrode changes under oxygen evolution conditions, turning from an oxide to an oxyhydroxide phase. Furthermore, the composition of the electrolyte has a significant effect on the oxygen evolution activity. We will discuss these results and their implications in finding better oxygen evolution electrocatalysts.

Biography.

John Kitchin completed his B.S. in Chemistry at North Carolina State University. He completed a M.S. in Materials Science and a PhD in Chemical Engineering at the University of Delaware in 2004 under the advisement of Dr. Jingguang Chen and Dr. Mark Barteau. He received an Alexander von Humboldt postdoctoral fellowship and lived in Berlin, Germany for 1 ½ years studying alloy segregation with Karsten Reuter and Matthias Scheffler in the Theory Department at the Fritz Haber Institut. Professor Kitchin began a tenure-track faculty position in the Chemical Engineering Department at Carnegie Mellon University in January of 2006. He is currently an Associate Professor. At CMU, Professor Kitchin is active in a major research effort within the National Energy Technology Laboratory Regional University Alliance in CO_2 capture,

chemical looping and superalloy oxidation. Professor Kitchin also uses computational methods to study adsorbate-adsorbate interactions on transition metal surfaces for applications in catalysis. He was awarded a DOE Early Career award in 2010 to investigate multifunctional oxide electrocatalysts for the oxygen evolution reaction in water splitting using experimental and computational methods. He received a Presidential Early Career Award for Scientists and Engineers in 2011.

Recent publications.

1. Sneha A. Akhade and John R. Kitchin*, "Effects of strain, d-band filling and oxidation state on the surface electronic structure and reactivity of 3d perovskite surface", J. Chem. Phys. 137, 084703 (2012).
2. James Landon, Ethan Demeter, Nilay İnoğlu, Chris Keturakis, Israel E. Wachs, Relja Vasić, Anatoly I. Frenkel, John R. Kitchin, "*Spectroscopic characterization of mixed Fe-Ni oxide electrocatalysts for the oxygen evolution reaction in alkaline electrolytes*", ACS Catalysis, 2, 1793-1801 (2012).
3. Sneha A. Akhade and John R. Kitchin*, Effects of strain, d-band filling and oxidation state on the bulk electronic structure of cubic 3d perovskites, J. Chem. Phys. 135, 104702 (2011).
4. N. Inoglu, and J.R. Kitchin, Identification of sulfur tolerant bimetallic surfaces using DFT parameterized models and atomistic thermodynamics, ACS Catalysis, 1, 399-407 (2011).

5. Isabela C. Man, Hai-Yan Su, Federico Calle-Vallejo, Heine A. Hansen, José I. Martínez, Nilay G. Inoglu, John Kitchin, Thomas F. Jaramillo, Jens K. Nørskov, Jan Rossmeisl, Universality in Oxygen Evolution Electro-Catalysis on Oxide Surfaces, ChemCatChem, 3, (2011).
6. Spencer D. Miller, Nilay İnoğlu, and John R. Kitchin, Configurational correlations in the coverage dependent adsorption energies of oxygen atoms on late transition metal fcc (111) surfaces, J. Chemical Physics, 134, 104709 (2011).
7. R. Chao, J. R. Kitchin, K. Gerdes, E. M. Sabolsky, and P. A. Salvador, Preparation of Mesoporous $La_{0.8}Sr_{0.2}MnO_3$ Infiltrated Coatings in Porous SOFC Cathodes Using Evaporation-Induced Self-Assembly Methods, ECS Transactions, 35 (1) 2387-2399 (2011).
8. W. Richard Alesi Jr., McMahan Gray, John R. Kitchin, CO_2 Adsorption on Supported Molecular Amidine Systems on Activated Carbon, ChemSusChem, 3(8), 948-956 (2010) Special issue on CO2 capture and Sequestration.
9. Nilay Inoglu, John R. Kitchin, Simple model explaining and predicting coverage-dependent atomic adsorption energies on transition metal surfaces, Physical Review B, 82, 045414 (2010).