Catalysis Club of Philadelphia

Thursday November 13, 2008
Holiday Inn Select Hotel
Naamans Road and I-95, Claymont, DE

Using Aberration-corrected STEM Imaging to Explore Chemical and Structural Variations in the MoVNbTeO Oxidation Catalyst

Prof. Douglas J. Buttrey
University of Delaware

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The Effect of Thermodynamic Properties of Zirconia-Supported Fe3O4 on Water-Gas Shift Activity

Ivan Baldychev
University of Pennsylvania
(Student Talk, 15 minutes)

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

Members: $30.00
Walk Ins & Non-members: $35.00
Student & Retired Members: $15.00

Menu
Chicken Champagne
Maryland Crab Cake *- Served with our own Remoulade Sauce*
Vegan *- Portabella Napolitano*

Meal reservations - Please notify your company representative or Alan Lee Stottlemyer (alan@udel.edu, phone: 302.831.6915, fax: 302.831.1048) by ***Thursday, November 6***.

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

Membership - Dues for the 2008-09 season will be $10.00 ($5.00 for the local chapter and $5.00 for the national club). Dues for students and post-docs will be $6.00 ($5.00 for local club and $1.00 for national club). Please send your payment to Steve Harris, Lyondell Chemical Co., 3801 West Chester Pike, Newtown Square, PA 19073-2387.

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Using Aberration-corrected STEM Imaging to Explore Chemical and Structural Variations in the MoVNbTeO Oxidation Catalyst

Prof. Douglas J. Buttrey

Center for Catalytic Science and Technology

Department of Chemical Engineering

University of Delaware, Newark, DE 19716

Abstract

Selective oxidation catalysis is used in production of roughly 25% of all important organic chemicals and intermediates used for making consumer and industrial products [1]. Current processes used to produce high-demand C3 derivatives, namely acrylic acid and acrylonitrile, make use of multicomponent bismuth molybdate catalysts with propene feeds [1-2]. Significant cost savings exist if propene can be replaced by propane as the feedstock. The dominant candidate for this process is based on the multiphase MoVTeNbO complex oxide system [1-3]. The best MoVTeNbO catalysts with respect to selectivity and activity are two-phase mixtures comprised of an orthorhombic network bronze phase (M1) and a hexagonal tungsten bronze (HTB)-type phase (M2) [2-3]. Structural models currently exist for both phases based on simultaneous Rietveld refinement of high-resolution synchrotron X-ray and neutron powder diffraction data [2]. Recently, we have used aberration-corrected STEM methods compare M1 phase preparations obtained from different synthetic routes. Structural models based on HAADF images are developed and compared to the refined model developed by DeSanto et al. (Figure 1(a)) [2-5].

As an extension of this work, we have characterized several compositional and structural variants. These include omission of Te and/or Nb, replacement of Nb with Ta [5,6], Te with Sb, and changing the basic framework structure. Understanding the relationship between crystal chemistry, stucture, and catalyst performance is a key concern in development of these catalysts.

References

[1] R. K. Grasselli, *Top. Catal.* **21** (2002) 79.

[2] P. DeSanto, D. J. Buttrey, R.K. Grasselli, , C. G. Lugmair, A. F. Volpe Jr., B. H. Toby, and T. Vogt, *Z. Krist*. **219** (2004) 152.

[3] W. D. Pyrz, D. A. Blom, T. Vogt, and D. J. Buttrey, *Angew. Chem., Int. Ed*. **47** (2008) 2788.

[4] W. D. Pyrz, D. A. Blom, V. V. Guliants, T. Vogt, and D. J. Buttrey, *J. Phys Chem C* **112** (2008) 10043.

[5] D. A. Blom, W. D. Pyrz, T. Vogt, and D. J. Buttrey, *J. Electr. Micr.* In press.

[6] P. DeSanto, D. J. Buttrey, R. K. Grasselli, W. D. Pyrz, C. G. Lugmair, A. F. Volpe, B. , T. Vogt, and B. H. Toby, *Top. Catal.* **38** (2006) 31.

[7] W. D. Pyrz, D. A. Blom, R. Shiju, V. V. Guliants, T. Vogt, and D. J. Buttrey, *Catal. Today* In press.

Speaker's Bio

Douglas J. Buttrey
Center for Catalytic Science and Technology
Department of Chemical Engineering
University of Delaware

Date and Place of Birth
October 31, 1954. Detroit, Michigan.

Education
1980 - 1984 Purdue University, Ph.D.
1976 - 1978 Purdue University, M.S.
1972 - 1976 Wayne State University, B.S.

Experience
Winter 2008 Visiting Professor, Catalysis Research Center, Hokkaido University, Sapporo, Japan (sabbatical)
Fall 2007 Visiting Professor, NanoCenter, University of South Carolina, Columbia SC (sabbatical)
2005-date University of Delaware, Professor of Chemical Engineering
1997-98 Brookhaven National Laboratory, Physics Department, Visiting Scientist (sabbatical)
1993-2005 University of Delaware, Associate Professor of Chemical Engineering
1987-93 University of Delaware, Assistant Professor of Chemical Engineering
1984-86 University of Cambridge, Post-Doctoral Fellow in Physical Chemistry

Fields of Research
Solid State Chemistry and Physics; Characterization of Electronic and Catalytic Materials; Structural Analysis; Thermodynamics and Phase Diagram Studies; Synthesis; Crystal Growth; Stoichiometry Control.

Professional
American Association for the Advancement of Science, American Chemical Society, American Institute of Chemical Engineers, Microscopy Society of America

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The Effect of Thermodynamic Properties of Zirconia-Supported Fe3O4 on Water-Gas Shift Activity

Ivan Baldychev

Department of Chemical Engineering

University of Pennsylvania

(Student Talk, 15 minutes)

Abstract

Thermodynamics of oxidation and reduction were investigated in connection with reactivity studies for a series of zirconia- and alumina-supported iron-oxide catalysts, using coulometric titration to measure oxidation isotherms. For all supported samples, from weight loadings of 5 wt% (one monolayer) up to 30 wt%, the Gibbs free energy of transition between Fe_2O_3 and Fe_3O_4 has decreased by factor of 2 compared to bulk iron oxide to -109 kJ/mole at 973 K. Water-Gas Shift (WGS) reaction rates on supported iron oxide have decreased by factor of 10 or more compared to bulk iron oxide, suggesting that the changes in thermodynamic properties are related to changed in catalytic properties.

Speaker's Bio

Ivan Baldychev received his bachelor degree of Chemical Engineering from University of Delaware and is currently a 3rd year Ph.D. student in the Department of Chemical Engineering at University of Pennsylvania, studying catalysis under Raymond Gorte and John Vohs.