

2010 Spring Symposium
The Catalysis Society of Metropolitan New York

Wednesday, March 17th, 2010

29 Trembley Drive
Asa Packer Campus, Lehigh University
Bethlehem, PA 18015

- 8:00 – 8:45 AM ***Registration and Continental Breakfast***
- 8:45 AM ***Opening Remarks***
 Marco J. Castaldi
 Columbia University
- 8:50 AM ***Welcome Remarks***
 Professor Bruce Koel
 Lehigh University
- 9:00 AM **Plenary Presentation – Catalytic Reforming of Fossil and Renewable
Fuels in Millisecond Reactors**
 Professor Lanny Schmidt
 University of Minnesota
- 9:45 AM **Global Kinetic Optimization of Water-Gas Shift Reactor Performance**
 Dr. Jeff Weisman
 Precision Combustion Inc.
- 10:15 AM **Catalytic Active Sites for H₂ Production from Bio-alcohols over
Transition Metal Oxide Nanoparticles**
 Professor Xianqin Wang
 New Jersey Institute of Technology
- 10:45 AM ***Coffee Break***

2010 Spring Symposium – Program

- 11:15 AM **Dynamic characterization of surfaces of Co/TiO₂ Fischer-Tropsch catalysts with infrared spectroscopy and DFT calculations**
Professor Simon Podkolzin
Stevens Institute
- 11:45 AM **Advancing the Catalysis Science of Practical Catalysts with Lehigh's New Cutting Edge Instrumentation**
Professor Israel Wachs
Lehigh University
- 12:15 PM ***Lunch***
- 1:30 – 3:00 PM **Poster Session**
- 3:00 PM **Controlling O-H, C-H, C-O, and C-C Bond Scission Sequence of Oxygenates: Theoretical Predictions and Experimental Verification**
Dr. Alan Stottlemyer
University of Delaware
- 3:30 PM **Reactions of CO+NO and CO+O on planar and faceted Ir(210): bridging the materials gap**
Dr. Wenhua Chen
Rutgers
- 4:00 PM **First principles guided design of borohydride oxidation electrocatalysts**
Professor Michael Janik
Penn State University
- 4:30 PM **Poster Awards**
- 4:45 PM ***Final Remarks***
- 5:00 PM ***Adjourn***

Posters

- 1. Structural Characterization of Vanadium Phosphate Catalysts Prepared using a Di-block Copolymer Template**
W. Weng, Z. Lin, N.F. Dummer, J.K. Bartley, G.J. Hutchings and C.J. Kiely
Department of Materials Science & Engineering, Lehigh University, Bethlehem, PA 18015, USA
- 2. The effect of potassium on the activity of Pt/CeO₂ catalyst for hydrogen production from ethylene glycol**
Zhong He, Xianqin Wang
Chemical, Biological and Pharmaceutical Engineering Department, New Jersey Institute of Technology
- 3. The Effect of Support on Redox Properties and Methanol-Oxidation Activity of Vanadia Catalysts**
Ivan Baldychev, John M. Vohs and Raymond J. Gorte
Department of Chemical & Biomolecular Engineering University of Pennsylvania Philadelphia, PA 19104
- 4. Surface Structure of Pd₃Fe(111) and Effects of Oxygen Adsorption**
Xiaofang Yang, Lindsey A. Welch, Jie Fu and Bruce E. Koel
Department of Chemistry, and Center for Advanced Materials and Nanotechnology, Lehigh University, Bethlehem, PA 18015 USA
- 5. Catalyst deactivation and regeneration studies reforming ethanol/gasoline blends containing sulfur**
Amanda Simson, Marco Castaldi, Bob Farrauto
Department of Earth and Environmental Engineering (HKSM), Columbia University, New York, NY (USA)
- 6. Model Based Prediction of Bimetallic Catalysts for Hydrogen Production from Ammonia Decomposition**
Danielle A. Hansgen, Jingguang G. Chen, Dionisios G. Vlachos
Chemical Engineering, University of Delaware

7. **In Situ Time Resolved Spectroscopic Studies of Metal Oxide Photocatalysts for Water Splitting**
Charles A. Roberts, Alexander A. Puzov, Somphonh Peter Phivilay,
and Israel E. Wachs
Department of Chemical Engineering, Lehigh University, Bethlehem, PA

8. **Copper Coordination in Cu-SSZ-13 and Cu-SSZ-16 Investigated by Variable-Temperature XRD**
Dustin W. Fickel and Raul F. Lobo
Center for Catalytic Science and Technology, Department of Chemical Engineering, University of Delaware, Newark, Delaware 19716

9. **New Insights into the Water-Gas Shift Reaction over Bulk $\text{Cr}_2\text{O}_3 \cdot \text{Fe}_2\text{O}_3$ Mixed Oxide Catalysts: A Combined *Operando* Raman-IR-MS Investigation**
Christopher Keturakis, Marco Daturi and Israel E. Wachs
Operando Molecular Spectroscopy and Catalysis Laboratory, Chemical Engineering Department, Lehigh University, Bethlehem, PA 18015 USA

10. **Nano-dispersed calcium oxide as a reversible and efficient CO_2 sorbent for temperatures between 300-500 °C**
Philipp Gruene, Marco J. Castaldi, Robert J. Farrauto
*Department of Earth and Environmental Engineering (HKSM)
Columbia University, New York, NY 10027*

11. **Kinetics of Adsorption and Reaction of Hydrocarbon Molecules on Ordered Sn/Pt(111) Alloy Surfaces**
Lindsey A. Welch, Bruce E. Koel
Lehigh University, Bethlehem, PA 18015

12. **Reaction pathways for ligand transfer and methylchlorosilane recombination on Cu(001)**
James Lallo, Everett Lee, Robin Lefkowitz, B.J. Hinch
Department of Chemistry, Rutgers University, Piscataway, NJ, 08854, USA

13. **Structure Property Relationships of Supported Pt/Ni Bimetallic Catalysts: Correlating the Extent of Pt-Ni Bimetallic Bond Formation with Low-Temperature Hydrogenation Activity**
W. Lonergan, D. G. Vlachos, J. G. Chen
Department of Chemical Engineering, University of Delaware

- 14. Catalyst by Design: Tuning the Selective Oxidation of CH₃OH to DMM over Supported V₂O₅/TiO₂/SiO₂ with TiO₂ Nanoligands**
Kevin F. Doura, Israel E. Wachs
Operando Molecular Spectroscopy and Catalysis Laboratory, Department of Chemical Engineering, Lehigh University, Bethlehem, PA 18015 USA
- 15. Thermodynamic Stability and Catalytic Activity of Heterogeneous Sites on Pd-ceria for Methane Oxidation**
Adam D. Mayernick, Michael J. Janik
Department of Chemical Engineering, Pennsylvania State University, University Park, PA 16802
- 16. Revealing Structure-Activity Relationships in Model Double-Supported WO_x/TiO₂/SiO₂ Solid Acid Catalysts by Atomic Scale Characterization**
Wu Zhou, Kevin F. Doura, Elizabeth I. Ross-Medgaarden, Israel E. Wachs and Christopher J. Kiely
Department of Materials Science and Engineering, Lehigh University, Bethlehem, PA 18015-3195, USA
- 17. Steam Reforming of Propane and Propylene over NiO and PtRh catalysts**
McKenzie P. Kohn, Marco J. Castaldi, Robert J. Farrauto
Columbia University, HKSM, New York, NY 10027 (USA)
- 18. Raman, UV-Vis, and IR-ATR study of Vanadium haloperoxidase Functional Mimics**
Julie E. Molinari and Israel E. Wachs
Lehigh University, Bethlehem, PA 18015 (USA)
- 19. Atomic Layer Deposition of Pt on WC for Fuel Cell Applications**
Irene J. Hsu, Daniel V. Esposito, Brian G. Willis, Jingguang G. Chen
Department of Chemical Engineering, University of Delaware, Newark, DE 19716
- 20. Fundamental Surface Structure-Photoactivity Relationships of Advanced Photocatalysts**
Somphonh Peter Phivilay and Israel E. Wachs
Department of Chemical Engineering, Lehigh University, Bethlehem, PA

21. **The impact of transport properties on a selective catalytic reactor: Preferential Oxidation of CO**
Federico Barra, Marco J. Castaldi
Earth and Environmental Engineering (Henry Krumb School of Mines)
Columbia University, New York, NY 10027

22. **Aging Study and Impacts of Sulfur During Autothermal Reforming of JP8 on Pt/Rh Catalyst**
Naomi Klinghoffer, Marco J. Castaldi
Department of Earth and Environmental Engineering, Columbia University, New York, NY 10027, USA

23. **STEM-HAADF Characterization of Au/ZnO Catalysts for CO Oxidation**
Q. He, A. Thomas, J.K. Edwards, A.F. Carley, G.J. Hutchings and C.J. Kiely
Department of Materials Science and Engineering, Lehigh University, Bethlehem, PA 18015-3195, USA

24. **Metal-Organic Frameworks Containing Open Metal Coordination Sites as Catalysts**
Yonggang Zhao, Moothetty Padmanabhan, Jing Li, Ankush Biradar, Tewodros (Teddy) Asefa
Department of Chemistry and Chemical Biology, Rutgers University
610 Taylor Road, Piscataway, NJ 08854

25. **Microstructure-Based Design for Replacing Rh with Co in a Synergistic Catalyst for the Reduction of NO with H₂**
Paul S. Dimick, Richard G. Herman, and Charles E. Lyman
Department of Chemical Engineering
Lehigh University, Bethlehem, PA 18015

26. **Pd-Multicore Encapsulated in Porous Silica Shell: Efficient and Recyclable Catalysts**
Yanfei Wang and Tewodros Asefa
Department of Chemical Engineering and Biochemical Engineering;
Department of Chemistry and Chemical Biology;
Rutgers, The State University of New Jersey, 610 Taylor Road, Piscataway NJ 08854, USA

- 27. Continuous Selective Henry Reaction Catalyzed by Amine-Supported Nanoporous Catalyst on Fixed-Bed Reactor**
Ankush V. Biradar and Tewodros Asefa
*Department of Chemical Engineering and Biochemical Engineering;
Department of Chemistry and Chemical Biology;
Rutgers, The State University of New Jersey, 610 Taylor Road, Piscataway NJ
08854, USA*
- 28. Reaction mechanism studies of cobalt-based Fischer-Tropsch catalysts with infrared spectroscopy and DFT calculations**
Jie Gao, Amrita Pal, Bert Weckhuysen, Simon Podkolzin
*Department of Chemical Engineering and Materials Science, Stevens Institute of
Technology.*
- 29. Identification and relative activity of molybdenum nanostructures for methane conversion to benzene with reaction kinetics, Raman spectroscopy and DFT calculations**
Bhairavi Modak, Jih-Mirn Jehng, Marie Badlissi, Munyee Wong, Jacqueline Rodriguez, Israel Wachs, Simon Podkolzin
*Department of Chemical Engineering and Materials Science, Stevens Institute of
Technology*
- 30. Solar-Driven bio-inspired inorganic catalyst for water oxidation**
G Charles Dismukes, Robin Brimblecombe, Annette Koo, Gerhard Swiegers,
and Leone Spiccia
*Department of Chemistry & Chemical Biology, Rutgers University, Piscataway,
NJ 08854*