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EDUCATION

UNIVERSITY OF WISCONSIN-MADISON, Madison, Wisconsin
Ph.D., Chemical Engineering, August 2008
Advisor: Professor James A. Dumesic

UNIVERSITY OF NOTRE DAME, Notre Dame, Indiana
B.S., Chemical Engineering, Magna Cum Laude, May 2003

RESEARCH INTERESTS

My research interests center around the investigation and development of heterogeneous catalytic systems through the use of reaction kinetics studies, characterization experiments, and kinetic modeling to elucidate the relationships between catalyst composition and function. The development of a potential catalytic system begins with reaction kinetics studies to determine activity, selectivity, stability, and kinetic features such as activation energies and reaction orders. Physical and chemical characterization experiments provide information regarding the nature of the active phases of the catalytic materials. Kinetic modeling can be used to determine mechanistic features of reaction pathways such as surface intermediates and kinetically-relevant elementary steps, and these models can also be used to survey the product distribution of a reaction over a broad range of process conditions. Integration of the information from all three of these areas provides insight into potential improvements for the catalytic system being studied. I plan to use the methodology described above to investigate and develop catalytic systems for the conversion of biomass-derived molecules to fuels and chemicals. These methods are particularly useful for biomass processing because it involves multiple reaction steps due to high oxygen content and degree of functionality. Understanding the fundamental relationships between the C-H, C-C, and C-O bond-breaking and bond-making events associated with conversion of biomass and the catalytic materials that perform these reactions is imperative to the development of catalytic systems with high activity, selectivity, and stability. This methodology is also appropriate for the development of new processes that take advantage of synergies within catalytic systems to simplify processing steps and increase activity and selectivity of catalytic materials, thereby reducing capital and operating costs associated with separation and purification steps. I am specifically interested in the areas of (i) C-C bond formation between carbohydrate-derived carbonyl-containing molecules for the production of fuel range hydrocarbons, (ii) chemical production via hydrogenolysis and oxidation of biomass-derived polyols, and (iii) light alkane upgrading via co-processing with biomass-derived oxygenates.

RESEARCH PUBLICATONS

1. Kunkes, E. L.; **Simonetti, D. A.**; West, R. M.; Serrano-Ruiz, J. C.; Gartner, C. A.; Dumesic, J. A.; Catalytic conversion of biomass to monofunctional hydrocarbons and targeted liquid-fuel classes. *Science* (2008), 322, 417-421.
2. **Simonetti, D. A.** and Dumesic, J. A. Catalytic production of liquid fuels from biomass-derived oxygenated hydrocarbons: catalytic coupling at multiple length scales. *Catalysis Reviews* (2009) 51(3), 441-484.
3. **Simonetti, D. A.** and Dumesic, J. A. Catalytic strategies for changing the energy content and achieving C-C coupling in biomass-derived oxygenated hydrocarbons. *ChemSusChem* (2008), 1, 725-733.
4. **Simonetti, D. A.**; Kunkes, E. L.; Rass-Hansen, J.; Soares, R. R.; Dumesic, J. A. Coupling of glycerol processing with Fischer-Tropsch synthesis for production of liquid fuels. *Green Chemistry* (2007), 9(10), 1073-1083.
5. **Simonetti, D. A.**; Kunkes, E. L.; Dumesic, J. A. Gas-phase conversion of glycerol to synthesis gas over carbon-supported platinum and platinum-rhenium catalysts. *Journal of Catalysis* (2007), 247(2), 298-306.
6. **Simonetti, D. A.**; Ahn, J. H.; Iglesia E. Selective C-C bond formation via methylative homologation with dimethyl ether for upgrading of alkanes on acidic zeolites. *In preparation for Journal of Catalysis.*
7. Soares, R. R.; **Simonetti, D. A.**; Dumesic, J. A. Glycerol as a source for fuels and chemicals by low-temperature catalytic processing. *Angewandte Chemie, International Edition* (2006), 45(24), 3982-3985.
8. Ferrin, P.; **Simonetti, D.** , Kandoi, S; Kunkes, E. ; Dumesic, J. A.; Norskov, J. K.; Mavrikakis, M. Modeling ethanol decomposition on transition metals: a combined application of scaling and Brønsted-Evans-Polanyi relations. *Journal of the American Chemical Society* (2009), 131(16), 5809-5815.
9. Kunkes, E. L.; **Simonetti, D. A.**; Dumesic, J. A.; Pryz, W. D.; Murillo, L. E.; Chen, J. G; Buttrey, D. J.; The role of rhenium in the conversion of glycerol to synthesis gas over carbon supported platinum-rhenium catalysts. *Journal of Catalysis* (2008), 260, 164-177.
10. Shabaker, J. W.; **Simonetti, D. A.**; Cortright, R. D.; Dumesic, J. A. Sn-modified Ni catalysts for aqueous-phase reforming: Characterization and deactivation studies. *Journal of Catalysis* (2005), 231(1), 67-76.
11. Kunkes, E. L.; Soares, R. R.; **Simonetti, D. A.**; Dumesic, J. A. An integrated catalytic approach for production of hydrogen by glycerol reforming coupled with water-gas-shift. *Applied Catalysis B: Environmental* (2009), 90, 693-698.
12. West, R. M.; Kunkes, E. L.; **Simonetti, D. A.**; Dumesic, J. A. Catalytic conversion of biomass-derived carbohydrates to fuels and chemicals by formation and upgrading of mono-functional hydrocarbon intermediates. *Catalysis Today* (2009), 147, 115-125.

13. Kharatyan, S. L.; Chatilyan, H. A.; Mukasyan, A. S.; **Simonetti, D. A.**; Varma, A. Effect of heating rate on kinetics of high-temperature reactions: Mo-Si system. *AIChE Journal* (2005), 51(1), 261-270.

CONFERENCE PRESENTATIONS

1. Ahn, J. H.; **Simonetti, D. A.**; Temel, B.; Iglesia, E. *"Homologation of dimethyl ether to highly branched alkanes on acidic zeolites"* 21st North American Catalysis Society Meeting, San Francisco, CA, June, 2009.
2. Ferrin, P.; **Simonetti, D. A.**; Kandoi, S.; Dumesic, J.; Norskov, J.; Mavrikakis, M. *"Reducing brute-force DFT work for surface reactivity by combining BEP and scaling relations"* 21st North American Catalysis Society Meeting, San Francisco, CA, June, 2009.
3. Kunkes, E. L.; Gurbuz, E. I.; Venvik, H. J.; **Simonetti, D. A.**; West, R. M.; Serrano-Ruiz, J. C.; Gaertner, C. A.; Dumesic, J. A. *"Catalytic conversion of carbohydrates to mono-functional hydrocarbons followed by catalytic C-C coupling"* 21st North American Catalysis Society Meeting, San Francisco, CA, June, 2009.
4. Ahn, J. H.; **Simonetti, D. A.**; Temel, B.; Iglesia, E. *"Mechanistic insights into the selective homologation of dimethyl ether to highly branched alkanes on acidic zeolites"* 237th American Chemical Society National Meeting, Salt Lake City, UT, March, 2009.
5. **Simonetti, D. A.**; Kunkes, E. L.; West, R. M.; Serrano-Ruiz, J. C.; Gartner, C. A.; Dumesic, J. A. *"Production of monofunctional hydrocarbons from biomass-derived carbohydrates via catalytic conversion on carbon supported Pt-Re catalysts."* 237th American Chemical Society National Meeting, Salt Lake City, UT, March, 2009.
6. **Simonetti, D. A.**; Kunkes, E. L.; West, R. M.; Serrano-Ruiz, J. C.; Gartner, C. A.; Dumesic, J. A. *"Catalytic conversion of biomass-derived polyols on carbon supported Pt-Re catalysts."* 2008 Pacific Coast Catalysis Society Meeting, Richmond, CA, November, 2008.
7. Kunkes, E. L.; **Simonetti, D. A.**; West, R. M.; Dumesic, J. A. *"Conversion of biomass-derived polyols over carbon supported Pt-Re catalysts"* 2008 AIChE Annual Meeting, Philadelphia, PA, November, 2008.
8. Ferrin, P. A.; **Simonetti, D. A.**; Kandoi, S.; Dumesic, J. A.; Norskov, J. K.; Mavrikakis, M. M. *"Catalytic ethanol decomposition: An example for reducing brute-force DFT work for surface reactivity by combining BEP and scaling relations"* 2008 AIChE Annual Meeting, Philadelphia, PA, November, 2008.
9. **Simonetti, D. A.**, Kunkes, E. L., Rass-Hansen, J., Soares, R. R., and Dumesic, J. A. *"Production of liquid fuels via catalytic glycerol processing coupled with Fischer-Tropsch synthesis."* 2007 AIChE Annual Meeting, Salt Lake City, UT, November, 2007.
10. **Simonetti, D. A.**, Kunkes, E. L., Rass-Hansen, J., Soares, R. R., and Dumesic, J. A. *"Liquid fuel and chemical production via coupled catalytic glycerol processing with Fischer-Tropsch synthesis."* Workshop on the Chemistry of Biomass Conversion to Biofuels, Biomaterials, and Chemicals. Brazilian Chemical Society Annual Meeting, Águas de Lindóia, São Paulo, Brazil, May, 2007.
11. Soares, R. R., **Simonetti, D. A.**, and Dumesic, J. A. *"Production of syngas or hydrogen by gas-phase reforming of aqueous glycerol solutions."* 14th Brazilian Catalysis Conference, Porto de Galinhas, Pernambuco, Brazil, September, 2007.
12. **Simonetti, D. A.**, Soares, R. R., and Dumesic, J. A. *"Glycerol as a source for fuels and chemicals by low-temperature catalytic processing."* 232nd American Chemical Society National Meeting, San Francisco, CA, September, 2006.
13. Soares, R. R., **Simonetti, D. A.**, and Dumesic, J. A. *"Fuels and chemicals from low-temperature catalytic conversion of glycerol to synthesis gas."* 2006 AIChE Annual Meeting, San Francisco, CA, November, 2006.

RESEARCH AND TEACHING EXPERIENCE

University of California-Berkeley, Berkeley, California
Postdoctoral Scholar, Research Group of Enrique Iglesia (July 2008 – present)
- Conducted kinetics experiments investigating methanol and dimethyl ether conversion on acid zeolite catalysts
- Conducted isotopic labeling studies to elucidate mechanistic details of carbon-carbon bond formation reactions
- Investigated the incorporation of H_2 into reaction products from methanol and dimethyl ether conversion on solid acids

University of Wisconsin-Madison, Madison, Wisconsin
Research Assistant, Research Group of James A. Dumesic (June 2003 – July 2008)
- Conducted kinetics experiments investigating catalytic reactions for the conversion of biomass-derived feedstocks
- Conducted characterization experiments to elucidate bulk and surface features of catalytic materials
- Constructed microkinetic models to determine essential kinetic features of reaction systems

University of Notre Dame, Notre Dame, Indiana
Undergraduate Research Assistant, Research Group of Arvind Varma (January 2002 – May 2003)
- Conducted kinetics experiments investigating combustion synthesis reactions of Mo-Si systems
- Performed scanning electron microscopy and x-ray diffraction experiments to characterize Mo-Si mixtures
- Investigated the effects of synthesis and purification processes on carbon nanotubes

University of Wisconsin-Madison, Madison, Wisconsin
Teaching Assistant, Transport Phenomena Laboratory; Chemical Kinetics and Reactor Design (September 2005 – May 2006)
- Prepared lectures describing the principles associated with transport phenomena and their applications
- Led weekly discussion sections emphasizing the fundamental principles of reactor design
- Evaluated laboratory reports, homework assignments, and exams

REFERENCES

Available upon request