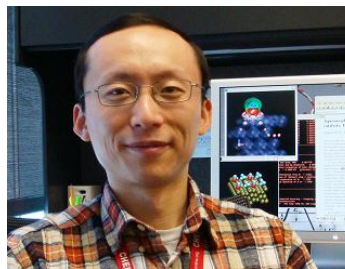


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Education

Massachusetts Institute of Technology	Chemical Engineering	B.S., 1999
University of Wisconsin-Madison	Chemical Engineering	Ph.D., 2004

Professional Experience

2006–p Research Staff Member, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory (ORNL)
2004–2006 Postdoctoral Research Associate, Computer Science and Mathematics Division (CSMD), ORNL

Professional and Synergistic Activities

2009–p Session Chair/Co-Chair, Computational Catalysis Session, American Institute of Chemical Engineers (AIChE) Annual Meetings
2009–p Proposal Reviewer: Argonne National Laboratory (ANL), Center for Nanoscale Materials (CNS); American Chemical Society (ACS)-Petroleum Research Funding Program (PRF); National Science Foundation (NSF); Department of Energy (DOE), Basic Office of Energy Sciences (BES)
2009 Session Chair, Catalysis in Fuel Chemistry Symposium, American Chemical Society Fall 2009 National Meeting & Exposition
2004–p Peer Reviewer: Journal for Physical Chemistry, Journal of American Chemical Society, Surface Science, Applied Catalysis, Catalysis Today, ACS Catalysis, Angewandte Chemie International Edition
2003–p Memberships: American Chemical Society, American Institute of Chemical Engineers, Electrochemical Society

Honors and Awards

2000 NSF Graduate Fellowship Honorable Mention
1999 Chemical Engineering Fellowship, University of Wisconsin-Madison

Recent Invited Talks

“Theoretical Insights into the Oxygen Reduction Reaction and the Selection of Transition Metal Electrocatalysts,” ECS Student Chapter, Georgia Institute of Technology, Atlanta, GA, April 2012.
“Theoretical Investigation of the Li-ORR Catalyzed by Metal Surfaces,” Division of Fuel Chemistry, 243rd ACS National Meeting & Exposition, San Diego, CA, March 2012.
“A Case Study in Computational Catalysis: Selective Activation of Methyl Acetate on Palladium Surfaces,” Southeastern Theoretical Chemistry Association Annual Meeting, University of South Carolina, Columbia, SC, May 2010.
“Selective Hydrogenolysis of Small Oxygenates on Transition Metal Surfaces,” Inaugural Jürgen Ladebeck Workshop on Computational Catalysis hosted by the Tri-State Catalysis Society and Sud Chemie, University of Kentucky, Lexington, KY, March 2010.

“Nano-Scale Environmental Effects on the Reactivity of Platinum Clusters,” Chemistry Department, Brookhaven National Laboratory, Upton, NY, March 2009.

Publications (27 publications including 3 book chapters) *Full list follows CV*

Research Synopsis

1. Theoretical and computational modeling applied to the investigation of surface/interfacial chemical thermodynamics and kinetics; reaction mechanisms; and material properties.
2. Heterogeneous catalysis and electrocatalysis on metals, metal compounds, and nano-materials.
3. Current focus: (i) selective conversion of biomass-derived compounds; (ii) electrochemical energy storage based on metal-air chemistry; (iii) size-defined clusters as novel catalysts.

Collaborations (Last 5 years; Outside ORNL)

Dr. R. R. Adzic (Brookhaven National Laboratory); Prof. M. Filler (Georgia Tech.); Prof. R. B. Getman (Clemson Univ.); Prof. V. V. Guliyants (Univ. of Cincinnati); Prof. G. W. Huber (Univ. of Massachusetts); Prof. M. Mavrikakis (Univ. of Wisconsin); Prof. W. F. Schneider (Univ. of Notre Dame); Prof. D. Sholl (Georgia Tech.).

Graduate and Postdoctoral Advisors and Advisees

Postdoctoral Advisor: Prof. W. F. Schneider (Univ. of Notre Dame); Dr. W. A. Shelton (ORNL)

Graduate Advisor: Prof. M. Mavrikakis (Univ. of Wisconsin-Madison)

Graduate and Postdoctoral Advisees

Postdoctoral (Current): Bradley Habenicht (ORNL); Gopi Kashna Phani Dathar (ORNL)

Postdoctoral (Previous): Lymarie Semidey-Flecha (Procter & Gamble); Lijun Xu (Univ. of VA)

PUBLICATIONS

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Book Chapters

- Y. Xu, "Recent Advances in Heterogeneous Catalysis Enabled by First-Principles Methods," Chapter 4, in *RSC Catalysis Book Series*, Vol. 21, Eds., J. J. Spivey and K. M. Dooley, RSC Publishing: Cambridge, United Kingdom (2009).
- Y. Xu, M. Shao, M. Mavrikakis, R. R. Adzic, "Recent Developments in the Electrocatalysis of the O₂ Reduction Reaction," Chapter 9 in *Fuel Cell Catalysis: A Surface Science Approach*, Vol. 1, Ed., M. Koper, Wiley: Somerset, New Jersey (2009).
- Y. Xu, W. A. Shelton, W. F. Schneider, "Theoretical Aspects of Oxide Particle Stability and Chemical Reactivity," Chapter 10 in *Synthesis and Application of Oxide Nanoparticles and Nanostructures*, Eds., J. A. Rodriguez, M. Fernández-García, Wiley: Somerset, New Jersey (2007).

Refereed Journal Articles

- K. Muthukumar, J. Yu, Y. Xu, V. V. Guliants, "Propane Ammoxidation over the Mo-V-Te-Nb-O M1 Phase: Reactivity of Surface Cations in Hydrogen Abstraction Steps," *Topics in Catalysis* **54**, 605 (2011).
- L. Xu and Y. Xu, "Effect of Pd Surface Structure on the Activation of Methyl Acetate," *Catalysis Today* **165**, 96 (2011).
- Y. Xu, L. Semidey-Flecha, L. Liu, Z. Zhou, D.W. Goodman, "Exploring the Structure and Chemical Activity of 2-D Gold Islands on Graphene Moiré/Ru(0001)," *Faraday Discussions* **152**, 267 (2011).
- Y. Xu and W. A. Shelton, "Oxygen Reduction by Lithium on Model Carbon and Oxidized Carbon Structures," *Journal of the Electrochemical Society* **158**, A1177 (2011).
- D. C. Ford, A. U. Nilekar, Y. Xu, M. Mavrikakis, "Partial and Complete Reduction of O₂ by Hydrogen on Transition Metal Surfaces," *Surface Science* **604**, 1565 (2010).
- A. Govindasamy, K. Muthukumar, J. Yu, Y. Xu, V. V. Guliants, "Adsorption of Propane, Isopropyl, and Hydrogen on Cluster Models of the M1 Phase of Mo-V-Te-Nb-O Mixed Metal Oxide Catalyst," *Journal of Physical Chemistry C* **114**, 4544 (2010).
- H. Olcay, L. Xu, Y. Xu, G. W. Huber, "Aqueous-Phase Hydrogenation of Acetic Acid over Transition Metal Catalysts," *ChemCatChem* **2**, 1420 (2010).
- Y. Xu and W.A. Shelton, "O₂ Reduction by Lithium on Au(111) and Pt(111)," *Journal of Chemical Physics* **133**, 024703 (2010).
- L. Xu and Y. Xu, "Activation of Methyl Acetate on Pd(111)," *Surface Science* **604**, 887 (2010).
- W. O. Gordon, Y. Xu, D. R. Mullins, S. H. Overbury, "Temperature Evolution of Structure and Bonding of Formic Acid and Formate on Fully Oxidized and Highly Reduced CeO₂(111)," *Physical Chemistry Chemical Physics* **11**, 11171 (2009).
- R. B. Getman, Y. Xu, W. F. Schneider, "Thermodynamics of Environment-Dependent Oxygen Adsorption on Pt (111)," *Journal of Physical Chemistry C* **112**, 9559 (2008).
- Y. Xu, R. B. Getman, W. A. Shelton, W. F. Schneider, "First-Principles Investigation of the Effect of Pt Cluster Size on CO and NO Oxidation Intermediates and Energetics," *Physical Chemistry Chemical Physics*, **10**, 6009 (2008).

- A. U. Nilekar, Y. Xu, J. Zhang, M. B. Vukmirovic, K. Sasaki, F. Uribe, R. R. Adzic, M. Mavrikakis, "Bimetallic and Ternary Alloys for Improved Oxygen Reduction Catalysis," *Topics in Catalysis* **46**, 276 (2007).
- Y. Xu, H. Marbach, R. Imbihl, I. G. Kevrekidis, M. Mavrikakis, "The Effect of Co-Adsorbed Oxygen on the Adsorption and Diffusion of Potassium on Rh(110): A First-Principles Study," *Journal of Physical Chemistry C* **111**, 7446 (2007).
- L. Grabow, Y. Xu, M. Mavrikakis, "Lattice Strain Effects on CO Oxidation on Pt(111)," *Physical Chemistry Chemical Physics* **8**, 3369 (2006).
- Y. Xu, W. A. Shelton, W. F. Schneider, "Effect of Particle Size on the Oxidizability of Platinum Clusters," *Journal of Physical Chemistry A* **110**, 5839 (2006).
- Y. Xu, W. A. Shelton, W. F. Schneider, "Thermodynamic Equilibrium Compositions, Structures, and Reaction Energies of Pt_xO_y ($x=1-3$) Clusters Predicted from First Principles," *Journal of Physical Chemistry B* **110**, 16591 (2006).
- D. C. Ford, Y. Xu, and M. Mavrikakis, "Atomic and Molecular Adsorption on Pt(111)," *Surface Science* **587**, 159 (2005).
- Y. Xu, J. Greeley, M. Mavrikakis, "Effect of Subsurface Oxygen on the Reactivity of the Ag(111) Surface," *Journal of the American Chemical Society* **127**, 12823 (2005).
- J. Zhang, M. B. Vukmirovic, Y. Xu, M. Mavrikakis, R. R. Adzic, "Controlling the Catalytic Activity of Platinum-Monolayer Electrocatalysts for Oxygen Reduction with Different Substrates," *Angewandte Chemie-International Edition* **44**, 2132 (2005).
- N. Lopez, T. V. W. Janssens, B. S. Clausen, Y. Xu, M. Mavrikakis, T. Bligaard, J. K. Nørskov, "On the Origin of the Catalytic Activity of Gold Nanoparticles for Low-Temperature CO Oxidation," *Journal of Catalysis* **223**, 232 (2004).
- Y. Xu, A. V. Ruban, M. Mavrikakis, "The Adsorption and Dissociation of O_2 on Pt-Co and Pt-Fe Alloys," *Journal of the American Chemical Society* **126**, 4717 (2004).
- Y. Xu and M. Mavrikakis, "Adsorption and Dissociation of O_2 on Gold Surfaces: Effect of Steps and Strain," *Journal of Physical Chemistry B* **107**, 9298 (2003).
- Y. Xu and M. Mavrikakis, "The Adsorption and Dissociation of O_2 Molecular Precursors on Cu: The Effect of Steps," *Surface Science* **538**, 219 (2003).
- J. K. Nørskov, T. Bligaard, A. Logadottir, S. Bahn, L. B. Hansen, M. Bollinger, H. Bengaard, B. Hammer, Z. Sljivancanin, M. Mavrikakis, Y. Xu, S. Dahl, C. J. H. Jacobsen, "Universality in Heterogeneous Catalysis," *Journal of Catalysis* **209**, 275 (2002).
- Y. Xu and M. Mavrikakis, "Adsorption and Dissociation of O_2 on Ir(111)," *Journal of Chemical Physics*, **116**, 10846 (2002).
- Y. Xu and M. Mavrikakis, "Adsorption and Dissociation of O_2 on Cu(111): Thermochemistry, Reaction Barrier and The Effect of Strain," *Surface Science* **494**, 131 (2001).