Ye Xu

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Education

Massachusetts Institute of Technology	Chemical Engineering	B.S. 1994
University of Wisconsin–Madison	Chemical Engineering	Ph.D. 2004
Oak Ridge National Laboratory	Postdoctoral Research	2004–2006

Professional Experience

2013–present	Assistant Professor, Cain Department of Chemical Engineering, Louisiana State University
2006–2013	Staff Scientist, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Recognitions

- NSF Graduate Fellowship Honorable Mention, 2000
- UW–Madison Chemical Engineering Departmental Fellowship, 1999

Journal Articles (Peer Reviewed)

50. S. Ma, Y. Wu*, J. Wang, Y. Zhang, Y. Zhang, X. Yan, Y. Wei, P. Liu, J. Wang, K. Jiang, S. Fan, Y. Xu, Z. Peng*, "Reversibility of noble metal-catalyzed aprotic Li-O*2* batteries," *Nano Lett.* **2015**, *15*, 8084-8090.

49. X. Xia*, J. Zhang, N. Lu, M.J. Kim, K. Ghale, Y. Xu, E. McKenzie, J. Liu, H. Ye, "Pd-Ir core-shell nanocubes: A type of highly efficient and versatile peroxidase mimic," *ACS Nano* **2015**, *9*, 9994-10004.

48. W.C. McKee, V. Meunier, Y. Xu*, "Reconciling the electronic and geometric corrugations of the hexagonal boron nitride and graphene nanomeshes," *Surf. Sci.* **2015**, *642*, L16-L19.

47. L. Guo, Y. Zhang, J. Wang, L. Ma, S. Ma, Y. Zhang, E. Wang*, Y. Bi, D. Wang, W.C. McKee, Y. Xu, J. Chen, Q.H. Zhang, C.W. Nan, L. Gu, P.G. Bruce*, Z. Peng*, "Unlocking the energy capabilities of micron-sized LiFePO4," *Nature Commun.* **2015**, *6*, 7898.

46. Z. Peng*, Y. Chen, P.G. Bruce, Y. Xu*, "Direct observation of the superoxide anion as a stable intermediate in the electro-reduction of oxygen in a non-aqueous electrolyte containing phenol as a proton source," *Angew. Chem. Inter. Ed.* **2015**, *54*, 8165-8168.

45. F.C. Calaza, T.-L. Chen, D.R. Mullins, Y. Xu, S.H. Overbury*, "Reactivity and reaction intermediates for acetic acid adsorbed on CeO_2(111)," *Catal. Today* **2015**, *253*, 65-76.

44. M. Yang, S. Li, Y. Wang, J.A. Herron, Y. Xu, L.F. Allard, S. Lee, J. Huang, M. Mavrikakis, M. Flytzani-Stephanopoulos*, "Catalytically active Au-O(OH)$_x$- species stabilized by alkali ions on zeolites and mesoporous oxides," *Science* **2014**, *346*, 1498-1501.

43. C.A. Wolcott, I.X. Green, T.L. Silbaugh, Y. Xu, C.T. Campbell*, "Energetics of adsorbed CH_2 and CH on Pt(111) by calorimetry: The dissociative adsorption of diiodomethane," *J. Phys. Chem. C* **2014**, *118*, 29310-29321.

42. J. Yu, Y. Xu, V.V. Guliants*, "Propane ammoxidation over Mo-V-Te-Nb-O M1 phase investigated by DFT: Elementary steps of ammonia adsorption, activation and NH insertion into π-allyl intermediate," *Top. Catal.* **2014**, *57*, 1145-1151.

41. J.J. Spivey*, S.K. Katla, C.S.S.R. Kumar, K.M. Dooley, J.C. Flake, L.H. Haber, Y. Xu, M.C. Janik, S.B. Sinnott, Y.T. Cheng, T. Liang, D.S. Sholl, T.A. Manz, U. Diebold, G.S. Parkinson, D.A. Bruce, P.E. de Jongh, "Synthesis, characterization and computation of catalysts at the Center for Atomic-Level Catalyst Design," *J. Phys. Chem. C* **2014**, 118, 20043-20069.

40. J. Yu, Y. Xu*, V.V. Guliants*, "Propane ammoxidation over Mo-V-Te-Nb-O M1 phase: Density functional theory study of propane oxidative dehydrogenation steps," *Catal. Today* **2014**, 238, 28-34.

39. M.C. Patterson, B.F. Habenicht, R.L. Kurtz, L. Liu, Y. Xu, P.T. Sprunger*, "Formation and stability of dense arrays of Au nanoclusters on hexagonal boron nitride/Rh(111)," *Phys. Rev. B* **2014**, 89, 205423.

38. T.L. Silbaugh, J.B. Giorgi, Y. Xu, A. Tillekaratne, F. Zaera, C.T. Campbell*, "Adsorption energy of tert-butyl on Pt(111) by dissociation of tert-butyl iodide: Calorimetry and DFT," *J. Phys. Chem. C* **2014**, *118*, 427-438.

37. H. Olcay, Y. Xu*, G.W. Huber*, "Effects of hydrogen and water on the activity and selectivity of acetic acid hydrogenation on ruthenium," *Green Chem.* **2014**, *16*, 911-924.

36. B.F. Habenicht, D. Teng, L. Semidey-Flecha, D.S. Sholl, Y. Xu*, "Adsorption and diffusion of 4d and 5d metal adatoms on graphene moiré/Ru(0001) and the implications for cluster nucleation," *Top. Catal.* **2014**, *57*, 69-79.

35. G.K.P. Dathar, Y.T. Tsai, K. Gierszal, Y. Xu, C. Liang, A. Rondinone, S.H. Overbury, V. Schwartz*, "Identifying active functionalities on few-layered graphene catalysts for oxidative dehydrogenation of isobutane," *ChemSusChem* **2014**, *7*, 483-491.

34. L. Semidey-Flecha, D. Teng, B.F. Habenicht, D.S. Sholl, Y. Xu*, "Adsorption and diffusion

of the Rh and Au adatom on graphene moiré/Ru(0001)," *J. Chem. Phys.* **2013**, *138*, 184710.

33. J. Lee, Y. Xu, G.W. Huber*, "High-throughput screening of monometallic catalysts for aqueous-phase hydrogenation of biomass-derived oxygenates," *Appl. Catal. B* **2013**, *140-141*, 98-107.

32. Z. Zhou, B.F. Habenicht, Q. Guo, Z. Yan, Y. Xu, L. Liu*, D.W. Goodman, "Graphene moiré structure grown on a pseudomorphic metal overlayer supported on Ru(0001)," *Surf. Sci.* **2013**, *611*, 67-73.

31. F.C. Calaza, Y. Xu, D.R. Mullins, S.H. Overbury*, "Oxygen vacancy-assisted coupling and enolization of acetaldehyde on CeO_2(111)," *J. Am. Chem. Soc.* **2012**, *134*, 18034-18045.

30. J. Yu, J. Woo, A. Borisevich, Y. Xu, V.V. Guliants*, "A combined HAADF STEM and DFT study of tantalum and niobium locations in the Mo-V-Te-Ta(Nb)-O M1 phases," *Catal. Commun.* **2012**, *29*, 68-72.

29. Y. Xu, "Decomposition of furan on Pd(111)," *Top. Catal*. **2012**, *55*, 290-299.

28. G.K.P. Dathar, W.A. Shelton, Y. Xu*, "Trends in the catalytic activity of transition metals for the oxygen reduction reaction by lithium," *J. Phys. Chem. Lett*. **2012**, *3*, 891-895.

27. 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 Discuss.* **2011**, *152*, 267-276.

26. Y. Xu* W.A. Shelton, "Oxygen reduction by lithium on model carbon and oxidized carbon structures," *J. Electrochem. Soc.* **2011**, *158*, A1177-A1184.

25. 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," *Top. Catal.* **2011**, *54*, 605-613.

24. L. Xu, Y. Xu*, "Effect of Pd surface structure on the activation of methyl acetate," *Catal. Today* **2011**, *165*, 96-105.

23. H. Olcay, L. Xu, Y. Xu*, G.W. Huber*, "Aqueous-phase hydrogenation of acetic acid over transition metal catalysts, *ChemCatChem* **2010**, *2*, 1420-1424.

22. D.C. Ford, A.U. Nilekar, Y. Xu*, M. Mavrikakis*, "Partial and complete reduction of O_2 by hydrogen on transition metal surfaces," *Surf. Sci.* **2010**, *604*, 1565-1575.

21. Y. Xu*, W.A. Shelton, "O_2 reduction by lithium on Au(111) and Pt(111)," *J. Chem. Phys.* **2010**, *133*, 024703.

20. L. Xu, Y. Xu*, "Activation of methyl acetate on Pd(111)," *Surf. Sci.* **2010**, *604*, 887-892.

19. A. Govindasamya, 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," *J. Phys. Chem. C* **2010**, *114*, 4544-4549.

18. 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 CeO_2(111)," *Phys. Chem. Chem. Phys.* **2009**, *11*, 11171-11183.

17. Y. Xu, R.B. Getman, W.A. Shelton, W.F. Schneider*, "A first-principles investigation of the effect of Pt cluster size on CO and NO oxidation intermediates and energetics," *Phys. Chem. Chem. Phys.* **2008**, *10*, 6009-6018.

16. R.B. Getman, Y. Xu, W.F. Schneider*, "Thermodynamics of environment-dependent oxygen adsorption on Pt(111)," *J. Phys. Chem. C* **2008**, *112*, 9559-9572.

15. 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," *Top. Catal.* **2007**, *46*, 276-284.

14. 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," *J. Phys. Chem. C* **2007**, *111*, 7446-7455.

13. 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," *J. Phys. Chem. B* **2006**, *110*, 16591-16599.

12. L. Grabow, Y. Xu, M. Mavrikakis*, "Lattice strain effects on CO oxidation on Pt(111)," *Phys. Chem. Chem. Phys.* **2006**, *8*, 3369-3374.

11. Y. Xu, W.A. Shelton, W.F. Schneider*, "Effect of particle size on the oxidizability of platinum clusters," *J. Phys. Chem. A* **2006**, *110*, 5839-5846.

10. Y. Xu, J. Greeley, M. Mavrikakis*, "Effect of subsurface oxygen on the reactivity of the Ag(111) surface," *J. Am. Chem. Soc.* **2005**, *127*, 12823-12827.

9. D.C. Ford, Y. Xu, M. Mavrikakis*, "Atomic and molecular adsorption on Pt(111)," *Surf. Sci.* **2005**, *587*, 159-174.

8. 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," *Angew. Chem. Int. Edit.* **2005**, *44*, 2132-2135.

7. Y. Xu, A.V. Ruban, M. Mavrikakis*, "The adsorption and dissociation of O_2 on Pt-Co and Pt-Fe alloys," *J. Am. Chem. Soc.* **2004**, *126*, 4717-4725.

6. 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," *J. Catal.* **2004**, *223*, 232-235.

5. Y. Xu, M. Mavrikakis*, "Adsorption and dissociation of O_2 on gold surfaces: Effect of steps and strain," *J. Phys. Chem. B* **2003**, *107*, 9298-9307.

4. Y. Xu, M. Mavrikakis*, "The adsorption and dissociation of O_2 molecular precursors on Cu: The effect of steps," *Surf. Sci.* **2003**, *538*, 219-232.

3. 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," *J. Catal.* **2002**, *209*, 275-278.

2. Y. Xu, M. Mavrikakis*, "Adsorption and dissociation of O_2 on Ir(111)," *J. Chem. Phys.* **2002**, *116*, 10846-10853.

1. Y. Xu, M. Mavrikakis*, "Adsorption and dissociation of O_2 on Cu(111): Thermochemistry, reaction barrier and the effect of strain," *Surf. Sci.* **2001**, *494*, 131-144.

Book Chapters (Peer Reviewed)

4. B.F. Habenicht, Y. Xu, L. Liu, "Graphene moiré supported metal clusters for model catalysis studies," in Graphene Chemistry: Theoretical Perspectives, ed. Z. Chen and D. Jiang; Wiley; **2013.**

3. Y. Xu, "Recent advances in heterogeneous catalysis enabled by first-principles methods," in RSC Catalysis series, ed. J.J. Spivey and K.M. Dooley. RSC; v. 21, **2009**.

2. Y. Xu, M. Shao, M. Mavrikakis, R.R. Adzic, "Recent developments in the electrocatalysis of the O_2 reduction reaction," in Fuel Cell Catalysis: A Surface Science Approach; ed. M.T.M. Koper. Wiley; **2009**.

1. Y. Xu, W.A. Shelton, W.F. Schneider, "Theoretical aspects of oxide particle stability and chemical reactivity," in Synthesis, Properties, and Applications of Oxide Nanomaterials; ed. J.A. Rodriguez, M. Fernández-Garcías. Wiley; **2007**.

Oral Presentations at Conferences (Y. Xu as speaker)

53. "Roles of oxygen vacancy in surface reactivity of CeO_2(111)," C. Zhao, Y. Xu, 249th ACS National Meeting, Denver, 03/2015.

52. "Reactivity of acetaldehyde on CeO_2(111) surfaces and the roles of oxygen vacancies," Y. Xu, 248th ACS National Meeting, San Francisco, 08/2014.

51. "Propane ammoxidation pathway over Mo-V-Te-Nb-O M1 phase catalyst probed by density functional theory calculations," Y. Xu, J. Yu, V.V. Guliants, 248th ACS National Meeting, San Francisco, 08/2014.

50. "Mechanistic insights into the electro-catalysis of Li-O_2 reduction & evolution reactions," G.K.P. Dathar, W.A. Shelton, Y. Xu, AIChE Annual Meeting, San Francisco, 11/2013.

49. "Reactivity of acetaldehyde on CeO_2(111) surfaces and the roles of oxygen vacancies," Y. Xu, AIChE Annual Meeting, San Francisco, 11/2013.

48. "Nanostructured gold model catalysts on oxygen-free substrates," L. Liu, F. Womack, Z. Zhou, M. Patterson, B.F. Habenicht, Y. Xu, P. Sprunger, R. Kurtz, AVS 60th Meeting, Long Beach, 10/2013.

47. "Reactivity of acetaldehyde on CeO_2(111) surfaces and the roles of oxygen vacancies," Y. Xu, F. Calaza, T.L. Chen, D.R. Mullins, S.H. Overbury, AVS 60th Meeting, Long Beach, 10/2013.

46. "Role of oxygen vacancy in the reactivity of acetaldehyde on CeO_2(111) Surfaces," Y. Xu, F. Calaza, T.-L. Chen, D.R. Mullins, S.H. Overbury, 246th ACS National Meeting, Indianapolis, 09/2013.

45. "Mechanistic insights into the electro-catalysis of Li-O_2 reduction & evolution reactions," G.K.P. Dathar, W.A. Shelton, Y. Xu, 246th ACS National Meeting, Indianapolis, 09/2013.

44. "Theoretical investigation of cathode materials for alternative lithium batteries," G.K.P. Dathar, W.A. Shelton, Y. Xu, 246th ACS National Meeting, Indianapolis, 09/2013.

43. "Aqueous-phase hydrogenation and hydrogenolysis of biomass-derived oxygenates over monometallic catalysts," J. Lee, Y. Xu, G.W. Huber, 246th ACS National Meeting, Indianapolis, 09/2013.

42. "DFT study of the mechanism of propane ammoxidation over Mo-V-Te-Nb-O M1 phase," J. Yu, Y. Xu, V.V. Guliants; 11th European Congress on Catalysis, Lyon, France, 09/2013.

41. "Locations of metal ions in Mo-V-Te-(Ta, Nb)-O M1 phases and their roles in propane ammoxidation to acrylonitrile," Y. Xu, V.V. Guliants, J. Woo, A. Borisevich; 11th European Congress on Catalysis, Lyon, France, 09/2013.

40. "Theoretical investigation of cathode catalysts for alternative Li batteries," Y. Xu, Symposium on Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors, 142nd The Minerals, Metals and Materials Society (TMS) Annual Meeting, San Antonio, 03/2013.

39. "Theoretical investigation of the oxygen reduction reaction by lithium catalyzed by metal surfaces," G.K.P. Dathar, W.A. Shelton, Y. Xu, Materials Research Society (MRS) Fall

Meeting, Boston, 12/2012.

38. "Oxygen vacancy-promoted coupling and enolization of acetaldehyde on CeO_2(111)," Y. Xu, F. Calaza, D.R. Mullins, S.H. Overbury, AIChE Annual Meeting, Pittsburgh, 10/2012.

37. "Catalytic activation of the O-C-O bond on transition metal surfaces," L. Xu, Y. Xu, AIChE Annual Meeting, Pittsburgh, 10/2012.

36. "A combined HAADF STEM and DFT study of tantalum and niobium location in the Mo-V-Te-Ta(Nb)-O M1 phase," J. Yu, J. Woo, A. Borisevich, Y. Xu, V.V. Guliants, AIChE Annual Meeting, Pittsburgh, 10/2012.

35. "Oxygen vacancy-promoted coupling and formation of enolate for acetaldehyde on CeO_2(111) surfaces," Y. Xu, F. Calaza, D.R. Mullins, S.H. Overbury, Southeastern Catalysis Society Annual Symposium, Asheville, 09/2012.

34. "Combining experiment and theory to improve understanding of surface reaction energetics and mechanisms," Y. Xu et al., Symposium on Progress in Electronic and Vibrational Spectroscopy of Catalytic Materials and Catalytic Reactions, 244th ACS National Meeting, Philadelphia, 08/2012.

33. "Theoretical investigation of the Li-ORR and OER catalyzed by metal surfaces," G.K.P. Dathar, W.A. Shelton, Y. Xu, 221st ECS Meeting, Seattle, 05/2012.

32. "Theoretical investigation of the Li-ORR catalyzed by metal surfaces," G.K.P. Dathar, W.A. Shelton, Y. Xu, Symposium on Theory and Simulation in Energy Production, Storage, and Utilization, 243rd ACS National Meeting, San Diego, 03/2012.

31. "Theoretical investigation of the oxygen reduction and redox activity of model carbon structures," G.K.P. Dathar, W.A. Shelton, Y. Xu, 243rd ACS National Meeting, San Diego, 03/2012.

30. "Selective conversion of carboxylic acids and esters on metallic catalysts," Y. Xu L. Xu, AIChE Annual Meeting, Minneapolis, 10/2011.

29. "A first-principles study of O_2 reduction by lithium on metal and carbon surfaces," Y. Xu, W.A. Shelton, Division of Fuel Chemistry, 242nd ACS National Meeting, Denver, 08/2011.

28. "Aqueous-phase hydrogenation of acetic acid on monometallic catalysts – A combined experimental and theoretical study," H. Olcay, L. Xu, Y. Xu, G.W. Huber, 22nd North American Catalysis Society (NACS) Meeting, Detroit, 06/2011.

27. "Exploring graphene moiré-supported clusters as a new catalytic material platform," D.W. Goodman, L. Liu, Z. Zhou, F. Gao, L. Semidey-Flecha, Y. Xu, D. Teng, D.S. Sholl, P. Sprunger, W. Plummer, Energy Frontier Research Centers Summit and Forum, Washington, 05/2011.

26. "A first-principles study of O_2 reduction by lithium on metal and carbon surfaces," Y. Xu, W.A. Shelton, 219th ECS Meeting, Montréal, 05/2011.

25. "First-principles study of the oxygen reduction reaction by lithium on metal and carbon surfaces," Y. Xu, W.A. Shelton, 241st ACS National Meeting, Anaheim, 03/2011.

24. "A first-principles study of O_2 reduction by lithium on metal and carbon surfaces," Y. Xu, W.A. Shelton, MRS Fall Meeting, Boston, 12/2010.

23. "Aqueous-phase hydrogenation of acetic acid on monometallic catalysts," H. Olcay, L. Xu, Y. Xu, G.W. Huber, AIChE Annual Meeting, Salt Lake City, 11/2010.

22. "Nano-scale environmental effects in the reactivity of platinum clusters," Y. Xu, Theory and Simulation of Nano-Scale Materials workshop, Sandia National Laboratory, 10/2010.

21. "A first-principles study of O_2 reduction by lithium on metal and carbon surfaces," Y. Xu, W.A. Shelton, 218th ECS Meeting, Las Vegas, 10/2010.

20. "Aqueous-phase hydrogenation of acetic acid on monometallic catalysts," H. Olcay, L. Xu, Y. Xu, G.W. Huber, Southeastern Catalysis Society Annual Symposium, Asheville, 09/2010.

19. "A first-principles study of O_2 reduction by lithium on various catalytic materials," Y. Xu, W.A. Shelton, 217th ECS Meeting, Vancouver, Canada, 04/2010.

18. "Selective hydrogenolysis of small oxygenates on transition metal surfaces," Y. Xu, L. Xu, 239th ACS National Meeting, San Francisco, 03/2010.

17. "A first-principles study of O_2 reduction by lithium on various catalytic materials," Y. Xu, W.A. Shelton, MRS Fall Meeting, Boston, 12/2009.

16. "A DFT study on the selective hydrogenation of acetic acid to ethanol on Ru," Y. Xu, AIChE Annual Meeting, Nashville, 11/2009.

15. "Aqueous-phase hydrogenation of acetic acid over transition metal catalysts: The role of the acetyl species," H. Olcay, Y. Xu, G.W. Huber, 21st NACS Meeting, San Francisco, 06/2009.

14. "Pathways and intermediates of formic acid decomposition on the CeO_2(111) surface," Y. Xu, W.O. Gordon, S.D. Senanayake, D.R. Mullins, S.H. Overbury, Somorjai Award Symposium, 237th ACS National Meeting, Salt Lake City, 03/2009.

13. "Selective hydrogenolysis of acetic acid to ethanol on Ru surfaces," Y. Xu, 237th ACS National Meeting, Salt Lake City, 03/2009.

12. "Aqueous-phase hydrogenation of acetic acid on late transition metal catalysts," Y. Xu, H. Olcay, G.W. Huber, AIChE Annual Meeting, Philadelphia, 11/2008.

11. "Nano-scale environmental effects in the reactivity of platinum clusters," Y. Xu, R.B. Getman, W.A. Shelton, W.F. Schneider, AIChE Annual Meeting, Philadelphia, 11/2008.

10. "Aqueous-phase hydrogenation of organic acids on mono metallic catalysts: a combined experimental and theoretical study," Y. Xu, H. Olcay, G.W. Huber, AIChE Annual Meeting, Salt Lake City, 11/2007.

9. "A first-principles investigation of the reactivity of cyclohexanes on iridium surfaces," Y. Xu D.E. Resasco, AIChE Annual Meeting, Salt Lake City, 11/2007.

8. "Nano-scale effects in the oxidation and the reactivity of platinum clusters," Y. Xu, W.A. Shelton, W.F. Schneider, AIChE Annual Meeting, San Francisco, 11/2006.

7. "Platinum clusters for oxidation catalysis: Nano-scale effects in thermodynamics and reactivity," Y. Xu, W.A. Shelton, W.F. Schneider, 232nd ACS National Meeting, San Francisco, 09/2006.

6. "DFT simulations of lean NO_x catalysis, R. Getman, W.F. Schneider," Y. Xu, 232nd ACS National Meeting, San Francisco, 09/2006.

5. "Platinum nanoclusters for oxidation catalysis: Thermodynamics, reactivity, and size dependence," Y. Xu, W.A. Shelton, W.F. Schneider, 231st ACS National Meeting, Atlanta, 03/2006.

4. "The oxidation of platinum clusters: Size dependence, thermodynamics, and effect on reactivity," Y. Xu, W.A. Shelton, W.F. Schneider, AIChE Annual Meeting, Cincinnati, 10/2005.

3. "Nano-scale effects in the oxidation of and adsorption on Pt clusters," Y. Xu, W.A. Shelton, W.F. Schneider, 19th NACS Meeting, Philadelphia, 05/2005.

2. "Wave propagation and promoter transport on catalytic surfaces: Quantum mechanics, experiments, and reaction/transport models," Y. Xu, H. Marbach, R. Imbihl, I.G. Kevrekidis, M. Mavrikakis, AIChE Annual Meeting, San Francisco, 11/2003.

1. "Trends in O_2 dissociation on platinum alloy surfaces based on first-principles calculations," Y. Xu, M. Mavrikakis, AIChE Annual Meeting, Indianapolis, 11/2002.

Invited Talks

22. "Complementing surface science experiment with theory for detailed understanding of surface reactivity of CeO_2(111)," Y. Xu, LSU Department of Chemistry Physical Chemistry Seminar, 11/2015.

21. "Complementing surface science experiment with theory for detailed understanding of surface reactions on CeO_2(111)," Y. Xu, Wilhelm Award Symposium in honor of Prof.

Manos Mavrikakis, AIChE Annual Meeting, Salt Lake City, Utah, 11/2015.

20. "Roles of oxygen vacancy in the surface reactivity of CeO_2(111)," Y. Xu, Symposium on Advances in Ceria Based Catalysis: Structural, Electronic and Chemical Properties Tailored for Chemical Conversion, 250th ACS National Meeting, Boston, Massachusetts, 08/2015.

19. "Surface reactivity of small organic oxygenates on CeO_2(111)," Y. Xu, Electroanalytical Chemistry Lecture Series, Changchun Institute of Applied Chemistry, Changchun, China, 06/2015.

18. "Roles of oxygen vacancy in the surface reactivity of CeO_2(111)," Southwestern Catalysis Society Annual Symposium, University of Houston, 04/2015.

17. "Mechanistic insights for propane ammoxidation over Mo-V-Te-Nb-O M1 phase from DFT and experiment," Distinguished Researcher Award Symposium in honor of Dr. James Burrington, 249th ACS National Meeting, Denver, 03/2015.

16. "Complementing experiment with theory for improved understanding of surface reactions," Department of Chemical and Biomolecular Engineering seminar, Clemson University, 12/2014.

15. "Theoretical investigation of cathode catalysts for alternative Li batteries," Symposium on Nanostructured Materials for Lithium Ion Batteries and for Supercapacitors, 142nd TMS Annual Meeting, San Antonio, 03/2013.

14. "Understanding surface processes through first-principles calculations," International Workshop on Acoustic Activation of Surface Processes, Breckenridge, 01/2013.

13. "Combining experiment and theory to improve understanding of surface reaction energetics and mechanisms," Symposium on Progress in Electronic and Vibrational Spectroscopy of Catalytic Materials and Catalytic Reactions, 244th ACS National Meeting, Philadelphia, 08/2012.

12. "Theoretical insights into the oxygen reduction reaction and the selection of transition metal electrocatalysts," Electrochemical Society Student Chapter, Georgia Institute of Technology, 04/2012.

11. "Theoretical investigation of the Li-ORR catalyzed by metal surfaces," Symposium on Theory and Simulation in Energy Production, Storage, and Utilization, 243rd ACS National Meeting, San Diego, 03/2012.

10. "A first-principles study of O_2 reduction by lithium on metal and carbon surfaces," Division of Fuel Chemistry, 242nd ACS National Meeting, Denver, 08/2011.

9. "Exploring the structure and chemical activity of 2-D gold islands on graphene moiré/Ru(0001)," Faraday Discussion 152: Gold, Cardiff University, UK, 07/2011.

8. "Understanding surface chemistry for energy applications via first-principles computation," School of Energy, Environmental, Biological & Medical Engineering, University of Cincinnati, 03/2011.

7. "A case study in computational catalysis: Selective activation of methyl acetate on palladium surfaces," Southeastern Theoretical Chemistry Association Annual Meeting, University of South Carolina, 05/2010.

6. "A first-principles study of O_2 reduction by lithium on various catalytic materials," Symposium on Research Opportunities in Electrochemical Energy Storage – Beyond Lithium Ion: Computational Perspectives, Argonne National Laboratory, 05/2010.

5. "Selective hydrogenolysis of small oxygenates on transition metal surfaces," Division of Fuel Chemistry, 239th ACS National Meeting, San Francisco, 03/2010.

4. "Selective hydrogenolysis of small oxygenates on transition metal surfaces," Inaugural Jürgen Ladebeck Workshop on Computational Catalysis, Tri-State Catalysis Society, Louisville, 03/2010.

3. "Selective hydrogenolysis of acetic acid to ethanol on Ru surfaces," Division of Catalysis Science and Technology, 237th ACS National Meeting, Salt Lake City, 03/2009.

2. "Nano-scale environmental effects on the reactivity of platinum clusters," Chemistry Department Seminar, Brookhaven National Laboratory, 03/2009.

1. "Insights for heterogeneous catalysis from first-principles calculations," Department of Chemical and Materials Engineering, University of Cincinnati, 01/2008.

Professional Activities

Reviewer

- Journals: *J. Phys. Chem., J. Chem. Phys., Angew. Chem. Int. Edit., J. Catal., Surf. Sci., ACS Catal., J. Am. Chem. Soc., Appl. Catal., Catal. Today, Nano Energy, Electrochem. Acta, Phys. Rev. Lett., Nature Commun., Nature Chem., Comp. Mater. Sci.*, *Accounts Chem. Res.*
- Research Proposals: for DOE-BES; NSF; ACS Petroleum Research Fund.
- User Proposal Review Panels: CNM (ANL); CFN (BNL); CNMS (ORNL).

Conference participation

- Organizer/co-organizer: Wilhelm Award Symposium in honor of Prof. Manos Mavrikakis (AIChE Annual Meeting, 2015); Symposium on Nano Catalysis (250th ACS National Meeting, 2015); Symposium on Surface Chemistry and Catalysis on Oxides (249th ACS National Meeting, 2015); Symposium on Integrating Theory and Experiment for Metal-Air Battery Systems (243th ACS National Meeting, 2012).

Workshop participation

- Invited participant: MGI Grand Challenges Summit (NIST/DOE, 2013); Future of Catalysis (SLAC/Stanford, 2012); Atomistic Simulations for Industrial Needs workshop (NIST, 2012); MGI workshop, (NIST/DOE, 2012); Computational Catalysis workshop (U. Notre Dame, 2010); Breaking the Chemical Barriers to Cellulosic Biofuels (DOE/NSF, 2007).

Graduate and Postdoctoral Advisors

Graduate – Manos Mavrikakis (U. Wisconsin–Madison)

Post-doctoral – William F. Schneider (U. Notre Dame); William A. Shelton (ORNL)

Thesis Advisor and Postgraduate-Scholar Sponsor

Former:

Post-doctoral researchers – Gopi Kashna Phani Dathar (Schrödinger); Bradley F. Habenicht (U. Cal.-Merced), Lymarie Semidey-Flecha (P&G), Lijun Xu (UOP)

Current (LSU):

Post-doctoral researcher – William C. McKee

Graduate Students – Chuanlin Zhao, Kushal Ghale, Xun Cheng, Saurin Rawal