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Professional Preparation

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|---------------------------------------|---------------|-------------------------|-------------------|
| Massachusetts Institute of Technology | Cambridge, MA | Chemical Engineering | B.S., 1999 |
| University of Wisconsin–Madison | Madison, WI | Chemical Engineering | Ph.D., 2004 |
| Oak Ridge National Laboratory | Oak Ridge, TN | Computational Chemistry | Postdoc., 2004–06 |

Appointments

| | |
|--------------|-----------------------------------------------------------------------------------------------------|
| 2019–present | Leon Pliner Distinguished Professor, Department of Chemical Engineering, Louisiana State University |
| 2019–present | Associate Professor, Department of Chemical Engineering, Louisiana State University |
| 2013–2019 | Assistant Professor, Department of Chemical Engineering, Louisiana State University |
| 2006–2013 | Staff Scientist, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory |

Journal Articles (Peer-Reviewed; *h*-index: 38 by Web of Science)

80. J. Liu, L. Guo*, Y. Xu, J. Huang, Z. Peng*, “K-O₂ electrochemistry at Au/DMSO interface probed by in situ spectroscopy and theoretical calculations,” *Faraday Discuss.* **2023**, doi: 10.1039/D3FD00071K
79. Md. S. Rahman, Y. Xu*, “Acetate formation on metals via CH₄ carboxylation by CO₂: A DFT study,” *Catal. Today* **2023**, *416*, 113891.
78. K. Nandakumar*, M. Tyagi, Y. Xu, K.T. Valsaraj, J.B. Joshi, “Chemical engineering at crossroads,” *Can. J. Chem. Eng.* **2022**, *100*, 2011-2027.
77. S. Bhasker-Ranganath, Y. Xu*, “Hydrolysis of acetamide on low-index CeO₂ surfaces: Ceria as a deamination and general de-esterification catalyst,” *ACS Catal.* **2022**, *12*, 10222-10234.
76. K. Viacheslav, Md.S. Rahman, L. Piliai, Y. Kosto, S.L. Mehl, T. Skála, I. Matolinová, V. Matolín, K.C. Prince, Y. Xu, N. Tsud*, “Thermal stability and protective properties of phenylphosphonic acid on Cu(111),” *Appl. Surf. Sci.* **2022**, *600*, 154036.
75. J. Wang*, L. Ma, J. Xu, Y. Xu, K. Sun*, Z. Peng*, “Oxygen electrochemistry in Li-O₂ batteries probed by in situ surface-enhanced Raman spectroscopy,” *SusMat* **2021**, *1*, 345-358.
74. F. McKay, Y. Fang, O. Kizilkaya, P. Singh, D.D. Johnson, A. Roy, D.P. Young, P.T. Sprunger, J.C. Flake, W.A. Shelton, Y. Xu*, “CoCrFeNi high entropy alloy as enhanced hydrogen evolution catalyst in an acidic solution,” *J. Phys. Chem. C* **2021**, *125*, 17008-17018.
73. S. Bhasker-Ranganath, Md.S. Rahman, C. Zhao, F. Calaza, Z. Wu, Y. Xu*, “Elucidating the mechanism of ambient-temperature aldol condensation of acetaldehyde on ceria,” *ACS Catal.* **2021**, *11*, 8621-8634.
72. S. Bhasker-Ranganath, C. Zhao, Y. Xu*, “Theoretical analysis of the adsorption of phosphoric acid and model phosphate monoesters on CeO₂(111),” *Surf. Sci.* **2021**, *705*, 121776.

71. S. Zhang, D.D. Johnson, W.A. Shelton, Y. Xu^{*}, “Hydrogen adsorption on ordered and disordered Pt-Ni alloys,” *Top. Catal.* **2020**, *63*, 714-727.
70. S. Bercha, S. Bhasker-Ranganath, X. Zheng, K. Beranová, M. Vorokhta, R.G. Acres, T. Skála, V. Matolín, K.C. Prince, Y. Xu, N. Tsud^{*}, “Adsorption structure of adenine on cerium oxide,” *Appl. Surf. Sci.* **2020**, *530*, 147257.
69. Z. Xi, X. Cheng, Z. Gao, M. Wang, T. Cai, M. Muzzio, E. Davidson, O. Chen, Y. Jung, S. Sun, Y. Xu^{*}, X. Xia^{*}, “Strain effect in palladium nanostructures as nanozymes,” *Nano Lett.* **2020**, *20*, 272-277.
68. S.H. Cho, J. Kim, J. Han^{*}, D. Lee, H.J. Kim, Y.T. Kim, X. Cheng, Y. Xu, J. Lee^{*}, E.E. Kwon^{*}, “Bioalcohol production from acidogenic products via a two-step process: A case study of butyric acid to butanol,” *Appl. Energy* **2019**, *252*, 113482.
67. Y. Fang, X. Cheng, J.C. Flake^{*}, Y. Xu^{*}, “CO₂ electrochemical reduction at thiolate-modified bulk Au electrodes,” *Catal. Sci. Technol.* **2019**, *9*, 2689-2701.
66. C. Zhao, C. Watt, P. Kent, S.H. Overbury, D.R. Mullins, F. Calaza^{*}, A. Savara^{*}, Y. Xu^{*}, “Coupling of acetaldehyde to crotonaldehyde on CeO_{2-x}(111): Bifunctional mechanism and role of oxygen vacancies,” *J. Phys. Chem. C* **2019**, *123*, 8273-8286.
65. W.C. McKee^{*}, S.H. Rawal, Y. Xu, “Efficiency enhancements of a restricted stochastic search algorithm for locating local and global minima,” *Chem. Phys. Lett.* **2019**, *725*, 1-7.
64. M. Abdel-Rahman, X. Feng, M. Muir, K. Ghale, Y. Xu, M. Trenary^{*}, “Reaction pathways for HCN on transition metal surfaces,” *Phys. Chem. Chem. Phys.* **2019**, *21*, 5274-5284.
63. W. Xu, C. Sun, K. Zhao, X. Cheng, S.H. Rawal, Y. Xu, Y. Wang^{*}, “Defect engineering activating (boosting) zinc storage capacity of MoS₂,” *Energy Stor. Mater.* **2019**, *16*, 527-534.
62. C. Zhao, Y. Xu^{*}, “Theoretical investigation of dephosphorylation of phosphate monoesters on CeO₂(111),” *Catal. Today* **2018**, *312*, 141-148.
61. R.G. Acres, X. Cheng, K. Ševčíková, S. Bercha, T. Skála, V. Matolín, Y. Xu, K.C. Prince, N. Tsud^{*}, “An experimental and theoretical study of adenine adsorption on Au(111),” *Phys. Chem. Chem. Phys.* **2018**, *20*, 4688-4698.
60. S.H. Rawal, W.C. McKee, Y. Xu^{*}, “Estimation of electric field effects on the adsorption of molecular metal superoxide species on Au based on density functional theory,” *Phys. Chem. Chem. Phys.* **2017**, *19*, 32626-32635.
59. S. Ma, W.C. McKee, J. Wang, L. Guo, E. Wang, M. Jansen, Y. Xu^{*}, Z. Peng^{*}, “Mechanistic origin of low polarization in aprotic Na-O₂ batteries,” *Phys. Chem. Chem. Phys.* **2017**, *19*, 12375-12383.
58. T. Duchoň^{*}, M. Aulická, E.F. Schwier, H. Iwasawa, C. Zhao, Y. Xu, K. Veltruská, K. Shimada, V. Matolín, “Covalent versus localized nature of 4f electrons in ceria: Resonant angle-resolved photoemission spectroscopy and density functional theory,” *Phys. Rev. B* **2017**, *95*, 165124.
57. A.J.R. Hensley, K. Ghale, C. Rieg, T. Dang, F. Studt, C.T. Campbell, J.-S. McEwen^{*}, Y. Xu^{*}, “A DFT-based method for more accurate adsorption energies: An adaptive sum of energies from RPBE and vdW density functionals,” *J. Phys. Chem. C* **2017**, *121*, 4937-4945.

56. C. Zhao, Y. Xu^{*}, “Simulated temperature programmed desorption of acetaldehyde on CeO₂(111): Evidence for the role of oxygen vacancy and hydrogen transfer,” *Top. Catal.* **2017**, *60*, 446-458.
55. W.C. McKee, M.C. Patterson, J.R. Frick, P.T. Sprunger, Y. Xu^{*}, “Adsorption of transition metal adatoms on *h*-BN/Rh(111): Implications for nanocluster self-assembly,” *Catal. Today* **2017**, *280P2*, 220-231.
54. L. Guo, L. Ma, Y. Zhang, X. Cheng, Y. Xu, J. Wang, E. Wang^{*}, Z. Peng^{*}, “Spectroscopic identification of the Au-C bond formation upon electroreduction of an aryl diazonium salt on gold,” *Langmuir* **2016**, *32*, 11514-11519.
53. Y. Zhang, Q. Cui, X. Zhang, W.C. McKee, Y. Xu, S. Ling, H. Li, G. Zhong, Y. Yang, Z. Peng^{*}, “Amorphous Li₂O₂: Chemical synthesis and electrochemical properties,” *Angew. Chem. Inter. Ed.* **2016**, *55*, 10717-10721.
52. W.C. McKee, M. Patterson, D. Huang, J. Frick, P. Sprunger, L. Liu^{*}, Y. Xu^{*}, “CO adsorption on Au nanoparticles grown on hexagonal boron nitride/Rh(111),” *J. Phys. Chem. C* **2016**, *120*, 10909-10918.
51. Y. Zhang, X. Zhang, J. Wang, W.C. McKee, Y. Xu, Z. Peng^{*}, “Potential-dependent generation of O₂⁻ and LiO₂ and their critical roles in O₂ reduction to Li₂O₂ in aprotic Li-O₂ batteries,” *J. Phys. Chem. C* **2016**, *120*, 3690-3698.
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-O₂ 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 CeO₂(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 CH₂ 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 CeO₂(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. Gulianti^{*}, “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 O₂ by hydrogen on transition metal surfaces,” *Surf. Sci.* **2010**, *604*, 1565-1575.
21. Y. Xu^{*}, W.A. Shelton, “O₂ 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. Govindasamy, K. Muthukumar, J. Yu, Y. Xu^{*}, V.V. Gulianti^{*}, “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 CeO₂(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.

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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 O₂ 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 O₂ 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 O₂ 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 O₂ on Ir(111),” *J. Chem. Phys.* **2002**, 116, 10846-10853.
1. Y. Xu, M. Mavrikakis*, “Adsorption and dissociation of O₂ on Cu(111): Thermochemistry, reaction barrier and the effect of strain,” *Surf. Sci.* **2001**, 494, 131-144.

Book Chapters

5. S. Bhasker-Ranganath, Y. Xu, “Recent mechanistic insights into some enzyme mimetic functions of ceria,” in *Emerging Materials and Environment*, ed. M. Shukla, E. Ferguson, and J. Leszczynski, Springer, **2023**.
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 v. 21*, ed. J.J. Spivey and K.M. Dooley, RSC, **2009**.

2. Y. Xu, M. Shao, M. Mavrikakis, R.R. Adzic, "Recent developments in the electrocatalysis of the O₂ 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**.

Invited Talks

33. "Theoretical investigation of the temperature-programmed reactivity of acetic acid on CeO₂(111)," Symposium on Bridging Surface Science to Catalysis, 265th American Chemical Society (ACS) National Meeting, Indianapolis, 03/2023.
32. "Theoretical investigation of ceria as a general de-esterification catalyst," ACS Southwest Regional Meeting, Baton Rouge, 11/2022
31. "Ceria as a versatile Lewis acid-base catalyst," Department of Chemical and Biological Engineering, University of Wisconsin-Madison, 11/2022.
30. "Theory as a bridge between surface science and catalysis," 263rd ACS National Meeting, San Diego, 03/2022.
29. "Interaction of small heteroatomic organic compounds with ceria," AVS 67th Virtual Symposium, 10/2021.
28. "Theoretical investigation of certain enzyme-mimetic functions of ceria," Symposium on Elucidation of Mechanisms and Kinetics on Surfaces, 261st ACS National Meeting (virtual), 04/2021.
27. "Theoretical investigation of the dephosphorylation of phosphates on ceria," 3rd Computational Chemistry/Computational Modeling Meeting, Vicksburg, 09/2019.
26. "Random alloys for fundamental electrocatalytic reactions," Gabor A. Somorjai Award Symposium in Honor of Manos Mavrikakis, 257th ACS National Meeting, Orlando, 04/2019.
25. "Mechanistic insights for C-C coupling of simple carbonyl compounds on CeO₂(111)," Symposium on Elucidation of Mechanisms and Kinetics on Surfaces, 257th ACS National Meeting, Orlando, 04/2019.
24. "Fundamental investigation of the surface reactivity of carbonyl compounds on ceria," Department of Chemical Engineering, University of Louisiana, 02/2019.
23. "Theoretical investigation of the reactivity of oxo compounds on ceria," US Army Engineer Research and Development Center, Vicksburg, 08/2018.
22. "Electric field effects on the stability of molecular superoxide intermediates in non-aqueous oxygen reduction reaction," Southeastern Theoretical Chemistry Association Annual Meeting, Louisiana State University, 05/2018.
21. "Theoretical investigation of the reactivity of oxo compounds on CeO₂(111)," 255th ACS National

Meeting, New Orleans, 03/2018.

20. "Mechanistic insights into non-aqueous metal-O₂ reduction reactions," Department of Chemical Engineering, University of South Carolina, 02/2017.
19. "Theoretical investigation of the reactivity of carbonyl compounds on CeO₂(111)," Symposium on Elucidation of Mechanisms and Kinetics on Surfaces, 251st ACS National Meeting, San Diego, 03/2016.
18. "Mechanistic insights for propane ammoxidation over Mo-V-Te-Nb mixed metal oxide M1 phase from density functional theory," Symposium on Surface Chemistry and Catalysis of Transition Metal Oxides, 251st ACS National Meeting, San Diego, 03/2016.
17. "Theoretical investigation of the oxygen reduction reaction in Li-O₂ batteries," Symposium on Application of Computational Chemistry for Energy and Fuel Production, 251st ACS National Meeting, San Diego, 03/2016.
16. "Complementing surface science experiment with theory for detailed understanding of surface reactivity of CeO₂(111)," Department of Chemistry Physical Chemistry Seminar, Louisiana State University, 11/2015.
15. "Complementing surface science experiment with theory for detailed understanding of surface reactions on CeO₂(111)," Wilhelm Award Symposium in Honor of Prof. Manos Mavrikakis, AIChE Annual Meeting, Salt Lake City, 11/2015.
14. "Roles of oxygen vacancy in the surface reactivity of CeO₂(111)," Symposium on Advances in Ceria Based Catalysis: Structural, Electronic and Chemical Properties Tailored for Chemical Conversion, 250th ACS National Meeting, Boston, 08/2015.
13. "Surface reactivity of small organic oxygenates on CeO₂(111)," Y. Xu, Electroanalytical Chemistry Lecture Series, Changchun Institute of Applied Chemistry, Changchun, China, 06/2015.
12. "Roles of oxygen vacancy in the surface reactivity of CeO₂(111)," Southwestern Catalysis Society Annual Symposium, Houston, 04/2015.
11. "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.
10. "Complementing experiment with theory for improved understanding of surface reactions," Department of Chemical and Biomolecular Engineering seminar, Clemson University, 12/2014.
9. "Understanding surface processes through first-principles calculations," International Workshop on Acoustic Activation of Surface Processes, Breckenridge, 01/2013.
8. "Theoretical insights into the oxygen reduction reaction and the selection of transition metal electrocatalysts," Electrochemical Society Student Chapter, Georgia Institute of Technology, 04/2012.
7. "Exploring the structure and chemical activity of 2-D gold islands on graphene moiré/Ru(0001)," Faraday Discussion 152: Gold, Cardiff University, United Kingdom, 07/2011.

6. "Understanding surface chemistry for energy applications via first-principles computation," School of Energy, Environmental, Biological & Medical Engineering, University of Cincinnati, 03/2011.
5. "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.
4. "A first-principles study of O₂ 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.
3. "Selective hydrogenolysis of small oxygenates on transition metal surfaces," Inaugural Jürgen Ladebeck Workshop on Computational Catalysis, Tri-State Catalysis Society, Louisville, 03/2010.
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.

Contributed Talks at Conferences (Y. Xu as speaker)

68. "A comparative study of size-dependent properties of nickel and cobalt nanoclusters on CeO₂(111)," Md.S. Rahman, T. Ara, Y. Xu, J. Zhou, Rocky Mountain Regional Meeting of ACS, Laramie, 09/2023.
66. "Theoretical investigation of ceria as a deamidation catalyst," S. Bhasker-Ranganath, Y. Xu, 264th ACS National Meeting, Chicago, 08/2022.
65. "Sum is better than the parts: CrCoFeNi high entropy alloy as hydrogen evolution catalyst in acidic solution," F. McKay, Y. Fang, A.N. Okafor, O. Kizilkaya, P. Singh, D.D. Johnson, A. Roy, D.P. Young, J.C. Flake, W.A. Shelton, P.T. Sprunger, Y. Xu, Southeastern Catalysis Society Annual Symposium, Atlanta, 02/2022.
65. "Hydrogen adsorption on ordered vs. disordered Pt-3d metal alloys," A. Okafor, S. Zhang, D.D. Johnson, W.A. Shelton, Y. Xu, 262nd ACS National Meeting (virtual), 08/2021.
64. "Theoretical investigation of methane carboxylation on metal surfaces," Md.S. Rahman, Y. Xu, 262nd ACS National Meeting (virtual), 08/2021.
63. "Theoretical investigation of the ketonization mechanism for acetic acid on CeO₂(111)," C. Zhao, Y. Xu, 26th NACS Meeting, Chicago, 06/2019.
62. "Mechanistic study on C-C coupling of acetaldehyde on partially reduced CeO_{2-x}(111)," C. Zhao, Y. Xu, AIChE Annual Meeting, Pittsburgh, 10/2018.
61. "Ligand-functionalized gold as versatile and tunable electrocatalysts for CO₂ reduction," Y. Fang, X. Cheng, Y. Xu, J.C. Flake, 254th ACS National Meeting, Washington, 08/2017.
60. "Fundamental investigation of C-C coupling of carbonyl compounds on ceria," C. Zhao, Y. Xu, 254th ACS National Meeting, Washington, 08/2017.

59. "Mechanistic insights into oxygen reduction reactions in non-aqueous metal-air batteries," Y. Zhang, X. Zhang, J. Wang, S. Ma, L. Guo, S. Rawal, W.C. McKee, Y. Xu, Z. Peng, 254th ACS National Meeting, Washington, 08/2017.
58. "Mechanistic insights into oxygen reduction and evolution reactions in non-aqueous metal-air batteries," Y. Zhang, X. Zhang, J. Wang, S. Ma, L. Guo, S. Rawal, W.C. McKee, Y. Xu, Z. Peng, 231th ECS Meeting, New Orleans, 05/2017.
57. "Enhanced electrocatalytic CO₂ reduction on thiol-functionalized gold," Y. Fang, X. Cheng, Y. Xu, J.C. Flake, AIChE Annual Meeting, San Francisco, 11/2016.
56. "The role of superoxide in the non-aqueous oxygen reduction reaction in Li-O₂ batteries," W.C. McKee, S. Rawal, Y. Xu, AIChE Annual Meeting, San Francisco, 11/2016.
55. "Enhanced electrocatalytic CO₂ reduction on thiol-functionalized gold," Y. Fang, X. Cheng, Y. Xu, J.C. Flake, 229th ECS Meeting, San Diego, 06/2016.
54. "Role of superoxide anion in the oxygen reduction reaction in non-aqueous electrolytes with a proton or lithium source," Y. Zhang, X. Zhang, J. Wang, Y. Chen, W.C. McKee, P.G. Bruce, Y. Xu, Z. Peng, 229th ECS Meeting, San Diego, 06/2016.
53. "Roles of oxygen vacancy in surface reactivity of CeO₂(111)," C. Zhao, Y. Xu, 249th ACS National Meeting, Denver, 03/2015.
52. "Reactivity of acetaldehyde on CeO₂(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. Guliyants, 248th ACS National Meeting, San Francisco, 08/2014.
50. "Mechanistic insights into the electro-catalysis of Li-O₂ reduction & evolution reactions," G.K.P. Dathar, W.A. Shelton, Y. Xu, AIChE Annual Meeting, San Francisco, 11/2013.
49. "Reactivity of acetaldehyde on CeO₂(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 International Symposium, Long Beach, 10/2013.
47. "Reactivity of acetaldehyde on CeO₂(111) surfaces and the roles of oxygen vacancies," Y. Xu, F. Calaza, T.L. Chen, D.R. Mullins, S.H. Overbury, AVS 60th International Symposium, Long Beach, 10/2013.
46. "Role of oxygen vacancy in the reactivity of acetaldehyde on CeO₂(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-O₂ 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 CeO₂(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 CeO₂(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 O₂ 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 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 O₂ 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 O₂ 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 O₂ 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 O₂ 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 O₂ 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 CeO₂(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 O₂ dissociation on platinum alloy surfaces based on first-principles calculations," Y. Xu, M. Mavrikakis, AIChE Annual Meeting, Indianapolis, 11/2002.

Professional Activities

Service

- Southwest Catalysis Society: Past-Chair (2019-2021), Chair (2018-2019), Chair-Elect (2017-2018), Director (2016-2017).
- LSU: ChE Awards and Events Committee (2019-present), ChE Graduate Committee (2017-2019, 2022-present), ChE Faculty Search Committee (2014-2016), College Distinguished Dissertation Selection Committee (2020, 2022), College Policy Committee (2014-2016), Materials Science and Engineering Committee (2018-present).

- Penn State UCFER: Core Competency Advisory Board (2019).

Reviewer

- Journals: *J. Phys. Chem.*, *J. Chem. Phys.*, *Phys. Chem. Chem. Phys.*, *Angew. Chem. Int. Edit.*, *J. Am. Chem. Soc.*, *Surf. Sci.*, *Appl. Surf. Sci.*, *J. Catal.*, *ACS Catal.*, *ChemCatChem*, *Appl. Catal.*, *Catal. Today*, *Top. Catal.*, *Catal. Sci. Technol.*, *Ind. Eng. Chem. Res.*, *Nano Energy*, *Electrochem. Acta*, *Phys. Rev. Lett.*, *Nature Commun.*, *Nature Chem.*, *Nature Catal.*, *Comp. Mater. Sci.*, *Accounts Chem. Res.*, *Appl. Phys. Lett.*
- Research proposals: DOE-BES; DOE-ARPA-E; NSF-CBET; NSF-Chemistry; ACS-PRF; Netherlands Organisation for Scientific Research; Research Council of Norway, National Research and Development Agency of Chile.
- User proposals: CNM (ANL); CNMS (ORNL); CFN (BNL).

Guest editor

- With L. Grabow: Catalytic Encounters at the Molecular Level: In Honor of Manos Mavrikakis, recipient of 2019 Gabor Somorjai Award for Creative Research in Catalysis, *Top. Catal.* **2020**, 63.
- With Y. Lei: A Decade of Effort in Addressing the Grand Challenges in Catalysis, *Catal. Today* **2017**, 280P2.
- With D.A. Bruce and J.J. Spivey: Special Section on Current Topics in Computational Catalysis, *Catal. Commun.* **2014**, 52.

Conference organization

- Symposium on Catalysis by Random/Complex/Disordered Alloys (264th ACS National Meeting, 2022); 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

- 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).

Recognitions

- NSF Graduate Fellowship Honorable Mention (2000).
- UW–Madison Chemical Engineering Departmental Fellowship (1999).

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

Graduate students – Andrew Okafor, Md. Saeedur Rahman, Suman Bhasker-Ranganath, Saurin H. Rawal, Xun Cheng, Kushal Ghale, Chuanlin Zhao

Post-doctoral researchers – William C. McKee, Gopi Kashna Phani Dathar; Bradley F. Habenicht, Lymarie Semidey-Flecha, Lijun Xu