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Hongliang Xin

Curriculum Vitæ

Education

2011 **Ph.D. in Chemical Engineering**, *University of Michigan, Ann Arbor*, MI.
Advisor: Prof. Suljo Linic
Dissertation: *First-principles Modeling of the Surface Reactivity of Transition Metals*

2005 **MSc in Chemical Engineering**, *Tsinghua University*, Beijing, China.
Advisor: Prof. Ming-han Han

2002 **BSc in Chemical Engineering**, *Tianjin University*, Tianjin, China.
Advisor: Prof. Shun-he Zhong

Academic Appointments

2020 **Associate Professor**, *Chemical Engineering, Virginia Tech.*

2014–2020 **Assistant Professor**, *Chemical Engineering, Virginia Tech.*

2013–2014 **Postdoctoral Research Fellow**, *Chemical Engineering, Stanford University/SLAC.*
Research areas: The d-band Theory of Chemisorption, Dynamic Modeling of Surface Reactions

2012–2013 **Postdoctoral Research Fellow**, *Chemical Engineering, University of Michigan, Ann Arbor.*
Research areas: Quantum-chemical Modeling of Plasmonic Catalysis, Fuel Cell Catalysis

Research Interests

- Machine Learning, Computational Chemistry, Multiscale Modeling
- Electronic Structure Theory, Catalysis Theory, Statistical Learning Theory
- Heterogeneous Catalysis, Electrocatalysis, Nonadiabatic Surface Chemistry
- CO_2 Reduction, NH_3 Synthesis, NH_3 Oxidation, NO_3^- Reduction

Honors & Awards

2020 **Jeffress Trust Award**, *The Thomas F. and Kate Miller Jeffress Memorial Trust.*

2019 **2019 Class Influential Researchers**, *ACS Industrial & Engineering Chemistry Research.*

2019 **Engineering Faculty Fellow Award**, *Virginia Tech College of Engineering.*

2019 **National Science Foundation CAREER.**

2018 **Outstanding New Assistant Professor Award**, *Virginia Tech College of Engineering.*

2017 **Journal of Materials Chemistry A - 2017 Emerging Investigators.**

2016 **NSF Travel Award for 16^{th} International Congress on Catalysis**, *Beijing, China.*

2016 **ICTAS Junior Faculty Award**, *Virginia Tech.*

2016 **Top Reviewer (2%)**, *ACS Catalysis.*

2015 **American Chemical Society PRF Doctoral New Investigator Award.**

2015 **Assistant Professor Mentoring Award**, *Virginia Tech, Blacksburg, VA.*

2011 **KOKES Award**, *22nd North American Catalysis Society Meeting, Detroit, MI.*

2011 **Weber Graduate Student Award in Environmental and Energy Sustainability**, *University of Michigan, Ann Arbor, MI.*

2008–2011 **Rackham Travel Award**, *University of Michigan, Ann Arbor, MI.*

2007 **Best Student Poster Award**, *Annual Symposium of the Michigan Catalysis Society, Ford Motor Company, Dearborn, MI.*

2002 **Sinopec Fellowship**, *Tianjin University, Tianjin, China.*

2001 **Rongzhijian Fellowship**, *Tianjin University, Tianjin, China.*

Publications at Virginia Tech

49 N. Omidvar and **H. Xin*** (Oct. 2021). "Algorithm-derived feature representations for explainable AI in catalysis". In: **Trends in Chemistry**. *doi: 10.1016/j.trechm.2021.10.001*.

48 S.-H. Wang, H. S. Pillai, S. Wang, L. E. K. Achenie, and **H. Xin*** (Sept. 2021). "Infusing theory into deep learning for interpretable reactivity prediction". In: **Nat. Commun.** 12.1, p. 5288. *doi: 10.1038/s41467-021-25639-8*.

47 J. Wang, Y. Lu, L. Liu, L. Yu, C. Yang, M. Delferro, A. S. Hoffman, S. R. Bare, A. Karim*, and **H. Xin*** (June 2021). "Catalytic CO Oxidation on $MgAl_2O_4$-Supported Iridium Single Atoms: Ligand Configuration and Site Geometry". In: **J. Phys. Chem. C** 125.21, pp. 11380–11390. *doi: 10.1021/acs.jpcc.1c02287*.

46 Y. Huang and **H. Xin*** (June 2021). "Ab initio machine learning for accelerating catalytic materials discovery". In: **Book: Catalysis**, pp. 347–379. *doi: 10.1039/9781839163128-00347*.

45 W. Wang, K. Wang, Z. Zhang, J. Chen, T. Mou, F. M. Michel, **H. Xin**, and W. Cai* (Mar. 2021). "Ultrahigh tribocorrosion resistance of metals enabled by nano-layering". In: **Acta Mater.** 206.116609, p. 116609. *doi: 10.1016/j.actamat.2020.116609*.

44 Y. Li, H. S. Pillai, T. Wang, S. Hwang, Y. Zhao, Z. Qiao, Q. Mu, S. Karakalos, M. Chen, J. Yang, D. Su, **H. Xin***, Y. Yan*, and G. Wu* (Jan. 2021). "High-Performance Ammonia Oxidation Catalysts for Anion-Exchange Membrane Direct Ammonia Fuel Cells". In: **Energy Environ. Sci.** *doi: 10.1039/D0EE03351K*.

43 Y. Rao, S. Wang, R. Zhang, S. Jiang, S. Chen, Y. Yu, S. Bao, M. Xu, Q. Yue, **H. Xin**, and Y. Kang* (Aug. 2020). "Nanoporous V-Doped Ni5P4 Microsphere: A Highly Efficient Electrocatalyst for Hydrogen Evolution Reaction at All pH". In: **ACS Appl. Mater. Interfaces** 12.33, pp. 37092–37099. *doi: 10.1021/acsami.0c08202*.

42 S. Wang, H. Pillai, and **H. Xin*** (2020). "Bayesian Learning of Chemisorption for Bridging the Complexity of Electronic Descriptors". In: **Nat. Commun.** *doi: 10.1038/s41467-020-19524-z*.

41 Q. Gao, T. Mou, S. Liu, G. Johnson, X. Han, Z. Yan, M. Ji, Q. He, S. Zhang, **H. Xin***, and H. Zhu* (Oct. 2020). "Monodisperse PdSn/SnOx core/shell nanoparticles with superior electrocatalytic ethanol oxidation performance". en. In: **J. Mater. Chem. A Mater. Energy Sustain.** 8.40, pp. 20931–20938. *doi: 10.1039/D0TA08693B*.

40 Z. Li, L. E. K. Achenie, and **H. Xin*** (Apr. 2020). "An Adaptive Machine Learning Strategy for Accelerating Discovery of Perovskite Electrocatalysts". In: **ACS Catal.** 10.7, pp. 4377–4384. *doi: 10.1021/acscatal.9b05248*.

39 Y. Li, X. Li, H. S. Pillai, J. Lattimer, N. Mohd Adli, S. Karakalos, M. Chen, L. Guo, H. Xu, J. Yang, D. Su, **H. Xin***, and G. Wu* (Apr. 2020). "Ternary PtIrNi Catalysts for Efficient Electrochemical Ammonia Oxidation". In: **ACS Catal.** 10.7, pp. 3945–3957. *doi: 10.1021/acscatal.9b04670*.

38 Q. Guan, C. Yang, S. Wang, L. He, Z. Kong, X. Chai, **H. Xin***, and P. Ning* (Oct. 2019). "Reactive Metal–Biopolymer Interactions for Semihydrogenation of Acetylene". In: **ACS Catal.** Pp. 11146–11152. *doi: https://doi.org/10.1021/acscatal.9b04042*.

37 K. Liu, **H. Xin**, and M. Han* (Sept. 2019). "Elucidation of key factors in nickel-diphosphines catalyzed isomerization of 2-methyl-3-butenenitrile". In: **J. Catal.** 377, pp. 13–19. *doi: https://doi.org/10.1016/j.jcat.2019.07.016*.

36 Z. Li, Z. Qi, S. Wang, T. Ma, L. Zhou, Z. Wu, X. Luan, F.-Y. Lin, M. Chen, J. T. Miller, **H. Xin***, W. Huang*, and Y. Wu* (Aug. 2019). "In Situ Formed Pt_3Ti Nanoparticles on a Two-Dimensional Transition Metal Carbide (MXene) Used as Efficient Catalysts for Hydrogen Evolution Reactions". In: **Nano Lett.** 19.8, pp. 5102–5108. *doi: https://doi.org/10.1021/acs.nanolett.9b01381*.

35 H. S. Pillai and **H. Xin*** (June 2019). "New Insights into Electrochemical Ammonia Oxidation on Pt(100) from First Principles". In: **Ind. Eng. Chem. Res.** 58.25, pp. 10819–10828. *doi: https://doi.org/10.1021/acs.iecr.9b01471*.

34 S. Wang and **H. Xin*** (Mar. 2019). "(Invited Preview) Predicting Catalytic Activity of High-Entropy Alloys for Electrocatalysis". In: **Chem** 5.3, pp. 502–504. *doi: https://doi.org/10.1016/j.chempr.2019.02.015*.

33 Z. Li, L. Yu, C. Milligan, T. Ma, L. Z. Zhou, Y. Cui, Z. Qi, B. Xu, J. Luo, E. Shi, Z. Wu*, **H. Xin***, W. N. Delgass, J. T. Miller*, and Y. Wu* (Dec. 2018). "Two-Dimensional Transition Metal Carbides (MXenes) as Supports for Tuning the Surface Chemistry of Catalytic Nanoparticles". In: **Nat. Commun.** 9.1, p. 5258. *doi: 10.1038/s41467-018-07502-5*.

32 Z. Li, S. Wang, and **H. Xin*** (Sept. 2018). "(Invited News & Views) Toward artificial intelligence in catalysis". In: **Nat. Catal.** 1.9, pp. 641–642. *doi: 10.1038/s41929-018-0150-1*.

31 S. Wang, N. Omidvar, E. Marx, and **H. Xin*** (Oct. 2018a). "Overcoming Site Heterogeneity In Search of Metal Nanocatalysts". In: **ACS Comb. Sci.** 20.10, pp. 567–572. *doi: 10.1021/acscombsci.8b00070*.

30 Y. Lu, J. Wang, L. Yu, L. Kovarik, X. Zhang, A. S. Hoffman, A. Gallo, S. R. Bare, D. Sokaras, T. Kroll, V. Dagle, **H. Xin***, and A. M. Karim* (Feb. 2019). "Identification of the active complex for CO oxidation over single-atom Ir-on-MgAl2O4 catalysts". In: **Nat. Catal.** 2.2, pp. 149–156. *doi: 10.1038/s41929-018-0192-4*.

29 Z. Li, N. Omidvar, W. S. Chin, E. Robb, A. Morris, L. Achenie, and **H. Xin*** (May 2018). "Machine Learning Energy Gaps of Porphyrins with Molecular Graph Representations". en. In: **J. Phys. Chem. A** 122.18, pp. 4571–4578. *doi: 10.1021/acs.jpca.8b02842*.

28 J. Wang, L. Yu, B. Hu, G. Chen, **H. Xin***, and X. Feng* (May 2018). "Efficient Electrohydrogenation of N_2 to NH_3 over Pd Catalyst at Low Overpotentials". In: **Nat. Commun.** 9.1, p. 1795. *doi: 10.1038/s41467-018-04213-9*.

27 S. Wang, N. Omidvar, E. Marx, and **H. Xin*** (Feb. 2018b). "Coordination numbers for unraveling intrinsic size effects in gold-catalyzed CO oxidation". en. In: **Phys. Chem. Chem. Phys.** 20.9, pp. 6055–6059. *doi: 10.1039/C8CP00102B*.

26 Z. Li, S. Wang, W. S. Chin, L. Achenie, and **H. Xin*** (2017). "High-throughput screening of bimetallic catalysts enabled by machine learning". en. In: **J. Mater. Chem. A Mater. Energy Sustain.** 5.46, pp. 24131–24138. *doi: 10.1039/C7TA01812F*.

25 S. Wang, J. Wang, and **H. Xin*** (Apr. 2017). "Insights into Electrochemical CO_2 Reduction on Tin Oxides from First-principles Calculations". In: **Green Energy & Environment** 2.2, pp. 168–171. *doi: 10.1016/j.gee.2017.02.005*.

24 W. Luc, C. Collins, S. Wang, **H. Xin**, K. He, Y. Kang, and F. Jiao* (Feb. 2017). "Ag-Sn Bimetallic Catalyst with a Core-Shell Structure for CO_2 Reduction". In: **J. Am. Chem. Soc.** 139.5, pp. 1885–1893. *doi: 10.1021/jacs.6b10435*.

23 Z. Li, X. Ma, and **H. Xin*** (Feb. 2017). "Feature Engineering of Machine-learning Chemisorption Models for Catalyst Design". In: **Catal. Today** 280, Part 2, pp. 232–238. *doi: 10.1016/j.cattod.2016.04.013*.

22 X. Ma and **H. Xin*** (Jan. 2017). "Orbitalwise Coordination Number for Predicting Adsorption Properties of Metal Nanocatalysts". In: **Phys. Rev. Lett.** 118.3, p. 036101. *doi: 10.1103/PhysRevLett.118.036101*.

21 **H. Xin*** and S. Linic* (June 2016). "Analyzing Relationships between Surface Perturbations and Local Chemical Reactivity of Metal Sites: Alkali Promotion of O_2 Dissociation on Ag(111)". In: **J. Chem. Phys.** 144.23, p. 234704. *doi: 10.1063/1.4953906*.

20 X. Ma, Z. Li, L. E. K. Achenie, and **H. Xin*** (Aug. 2015). "Machine-Learning-Augmented Chemisorption Model for CO_2 Electroreduction Catalyst Screening". In: **J. Phys. Chem. Lett.** Pp. 3528–3533. *doi: 10.1021/acs.jpclett.5b01660*.

19 X. Ma, J. S. A. Carneiro, X.-K. Gu, H. Qin, **H. Xin**, K. Sun, and E. Nikolla* (May 2015). "Engineering Complex, Layered Metal Oxides: High-Performance Nickelate Oxide Nanostructures for Oxygen Exchange and Reduction". In: **ACS Catal.** Pp. 4013–4019. *doi: 10.1021/acscatal.5b00756*.

Publications at Michigan, Stanford, and Tsinghua (China)

18 J. LaRue, O. Krejčı, L. Yu, M. Beye, M. L. Ng, H. Öberg, **H. Xin**, G. Mercurio, S. Moeller, J. J. Turner, D. Nordlund, R. Coffee, M. P. Minitti, W. Wurth, L. G. M. Pettersson, H. Öström, A. Nilsson, F. Abild-Pedersen, and H. Ogasawara (Aug. 2017). "Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru". In: **J. Phys. Chem. Lett.** 8.16, pp. 3820–3825. *doi: 10.1021/acs.jpclett.7b01549*.

17 M. Beye, H. Öberg, **H. Xin**, G. L. Dakovski, M. Dell'Angela, A. Föhlisch, J. Gladh, M. Hantschmann, F. Hieke, S. Kaya, D. Kühn, J. LaRue, G. Mercurio, M. P. Minitti, A. Mitra, S. P. Moeller, M. L. Ng, A. Nilsson, D. Nordlund, J. Nørskov, H. Öström, H. Ogasawara, M. Persson, W. F. Schlotter, J. A. Sellberg, M. Wolf, F. Abild-Pedersen, L. G. M. Pettersson, and W. Wurth (Sept. 2016). "Chemical Bond Activation Observed with an X-ray Laser". In: **J. Phys. Chem. Lett.** 7.18, pp. 3647–3651. *doi: 10.1021/acs.jpclett.6b01543*.

16 H. Öström, H. Öberg, **H. Xin**, J. LaRue, M. Beye, M. Dell'Angela, J. Gladh, M. L. Ng, J. A. Sellberg, S. Kaya, G. Mercurio, D. Nordlund, M. Hantschmann, F. Hieke, D. Kühn, W. F. Schlotter, G. L. Dakovski, J. J. Turner, M. P. Minitti, A. Mitra, S. P. Moeller, A. Föhlisch, M. Wolf, W. Wurth, M. Persson, J. K. Nørskov, F. Abild-Pedersen, H. Ogasawara, L. G. M. Pettersson, and A. Nilsson* (Feb. 2015). "Probing the Transition State Region in Catalytic CO Oxidation on Ru". In: **Science** 347.6225, pp. 978–982. *doi: 10.1126/science.1261747*.

15 **H. Xin**, J. LaRue, H. Öberg, M. Beye, M. Dell'Angela, J. J. Turner, J. Gladh, M. L. Ng, J. A. Sellberg, S. Kaya, G. Mercurio, F. Hieke, D. Nordlund, W. F. Schlotter, G. L. Dakovski, M. P. Minitti, A. Föhlisch, M. Wolf, W. Wurth, H. Ogasawara, J. K. Nørskov, H. Öström, L. G. M. Pettersson, A. Nilsson, and F. Abild-Pedersen* (Apr. 2015). "Strong Influence of Coadsorbate Interaction on CO Desorption Dynamics on Ru(0001) Probed by Ultrafast X-Ray Spectroscopy and *Ab Initio* Simulations". In: **Phys. Rev. Lett.** 114.15, p. 156101. *doi: 10.1103/PhysRevLett.114.156101*.

14 M. J. Kale, T. Avanesian, **H. Xin**, J. Yan, and P. Christopher* (2014). "Controlling Catalytic Selectivity on Metal Nanoparticles by Direct Photoexcitation of Adsorbate–Metal Bonds". In: **Nano Lett.** 14.9, pp. 5405–5412. *doi: 10.1021/nl502571b*.

13 **H. Xin**, A. Vojvodic, J. Voss, J. K. Nørskov, and F. Abild-Pedersen* (Mar. 2014). "Effects of *d*-band Shape on the Surface Reactivity of Transition-Metal Alloys". In: **Phys. Rev. B** 89.11, p. 115114. *doi: 10.1103/PhysRevB.89.115114*.

12 S. Linic*, P. Christopher, **H. Xin**, and A. Marimuthu (2013). "Catalytic and Photocatalytic Transformations on Metal Nanoparticles with Targeted Geometric and Plasmonic Properties". In: **Acc. Chem. Res.** 46.8, pp. 1890–1899. *doi: 10.1021/ar3002393*.

11 A. Holewinski, **H. Xin**, E. Nikolla, and S. Linic* (Aug. 2013). "Identifying Optimal Active Sites for Heterogeneous Catalysis by Metal Alloys based on Molecular Descriptors and Electronic Structure Engineering". In: **Curr. Opin. Chem. Eng.** 2.3, pp. 312–319. *doi: 10.1016/j.coche.2013.04.006*.

10 P. Christopher, **H. Xin**, A. Marimuthu, and S. Linic* (Dec. 2012). "Singular Characteristics and Unique Chemical Bond Activation Mechanisms of Photocatalytic Reactions on Plasmonic Nanostructures". In: **Nat Mater** 11.12, pp. 1044–1050. *doi: 10.1038/nmat3454*.

9 **H. Xin**, A. Holewinski, N. Schweitzer, E. Nikolla, and S. Linic* (June 2012). "Electronic Structure Engineering in Heterogeneous Catalysis: Identifying Novel Alloy Catalysts Based on Rapid Screening for Materials with Desired Electronic Properties". In: **Top Catal** 55.5-6, pp. 376–390. *doi: 10.1007/s11244-012-9794-2*.

8 **H. Xin**, A. Holewinski, and S. Linic* (Jan. 2012). "Predictive Structure–Reactivity Models for Rapid Screening of Pt-Based Multimetallic Electrocatalysts for the Oxygen Reduction Reaction". In: **ACS Catal.** 2.1, pp. 12–16. *doi: 10.1021/cs200462f*.

7 P. Christopher, **H. Xin**, and S. Linic* (June 2011). "Visible-light-enhanced Catalytic Oxidation Reactions on Plasmonic Silver Nanostructures". In: **Nat Chem** 3.6, pp. 467–472. *doi: 10.1038/nchem.1032*.

6 **H. Xin** and S. Linic* (June 2010). "Communications: Exceptions to the *d*-band Model of Chemisorption on Metal Surfaces: The Dominant Role of Repulsion between Adsorbate States and Metal d-states". In: **J. Chem. Phys.** 132.22, pp. 221101–221101–4. *doi: 10.1063/1.3437609*.

5 **H. Xin**, N. Schweitzer, E. Nikolla, and S. Linic* (Mar. 2010). "Communications: Developing Relationships between the Local Chemical Reactivity of Alloy Catalysts and Physical Characteristics of Constituent Metal Elements". In: **J. Chem. Phys.** 132.11, pp. 111101–111101–4. *doi: 10.1063/1.3336015*.

4 N. Schweitzer, **H. Xin**, E. Nikolla, J. T. Miller, and S. Linic* (Feb. 2010). "Establishing Relationships Between the Geometric Structure and Chemical Reactivity of Alloy Catalysts Based on Their Measured Electronic Structure". In: **Top Catal** 53.5-6, pp. 348–356. *doi: 10.1007/s11244-010-9448-1*.

3 Q. Wu, M.-H. Han*, **H. Xin**, B.-Q. Dong, and Y. Jin (Feb. 2008). "Studies on IR Spectroscopy and Quantum Chemical Calculation of Chloroaluminate Ionic Liquids Acidity". In: **Guang Pu Xue Yu Guang Pu Fen Xi** 28.2, pp. 282–284.

2 Q. Wu, B.-Q. Dong, M.-H. Han*, **H. Xin**, Y.-Z. Zuo, and Y. Jin (Mar. 2007). "Studies on Acidity of Cloroaluminate Ionic Liquids and its Catalytic Performance for Alkylation of Benzene with Long-chain Alkenes". In: **Guang Pu Xue Yu Guang Pu Fen Xi** 27.3, pp. 460–464.

1 **H. Xin**, Q. Wu, M. Han*, D. Wang, and Y. Jin (Sept. 2005). "Alkylation of Benzene with 1-dodecene in Ionic Liquids $[Rmim]^{+}Al_2Cl_6X^{-}$ (R = butyl, octyl and dodecyl; X = chlorine, bromine and iodine)". In: **Appl. Catal., A** 292, pp. 354–361. *doi: 10.1016/j.apcata.2005.06.012*.

Invited Lectures and Presentations

51. **H. Xin***, "Interpretable Machine Learning for Accelerating Catalytic Materials Discovery", **SUNCAT ML Workshop**, Virtual, 09/2021

50. **H. Xin***, "Bayesian Learning Reveals the Nature of Chemical Bonding at Single Atom Alloys", **ACS Fall Meeting**, in honor of Phil Christopher in Catalysis Award, Atlanta, 8/2021

49. **H. Xin***, "Interpretable Machine Learning of Chemical Bonding at Solid Surfaces", **ACS Fall Meeting**, Atlanta, 8/2021

48. **H. Xin***, "Theory-infused Neural Networks (TinNet) for Interpretable Reactivity Prediction", **"Computational Materials Chemistry" Telluride Workshop**, Virtual, 07/2021
47. **H. Xin***, "Interpretable Machine Learning for Accelerating Catalytic Materials Discovery", **Northwestern University**, Virtual, 06/2021
46. **H. Xin***, "Theory-infused Machine Learning Algorithms of Chemisorption at Metal Surfaces", **TMS2021**, Virtual, 03/2021
45. **H. Xin***, "Infusing Theory into Machine Learning for Catalysis", **Kansas State University**, Manhattan, KS, 12/2020
44. **H. Xin***, "Accelerating Discovery of High-Performance Electrocatalysts for Ammonia Oxidation Reaction Via Machine Learning", **AIChE Annual Virtual Meeting**, 11/2020
43. **H. Xin***, "Bayesian Learning of Chemisorption for Bridging the Complexity of Electronic Descriptors", **AIChE Annual Virtual Meeting**, 11/2020
42. **H. Xin***, "Physics Informed Machine Learning of Chemisorption at Metal Surfaces", **AIChE Annual Virtual Meeting**, 11/2020
41. **H. Xin***, "Bayesian Chemisorption Model for Adsorbate-Specific Tuning of Electrocatalysis", **ACS Spring Virtual Meeting**, 4/2020
40. **H. Xin***, Z. Li, S. Wang, and N. Omidvar, "Advancing Catalysis Theory and Catalyst Discovery via Ab Initio Machine Learning", **NAM 26**, Chicago, IL, 6/2019
39. S. Wang, and **H. Xin***, "Bayesian Chemisorption Theory of Catalysis", **ACS Spring Meeting**, Orlando, FL, 4/2019
38. Zheng Li, S. Wang, and **H. Xin***, "Machine Learning for Accelerating Discovery of Perovskite Electrocatalysts", **ACS Spring Meeting**, Orlando, FL, 4/2019
37. **J. Wang***, and H. Xin, "Machine Learning Molecular Dynamics for Understanding Nonadiabatic Surface Reactions", **AIChE Annual Meeting**, Pittsburgh, PA, 11/2018
36. **S. Wang***, and H. Xin, "Overcoming Site Heterogeneity in Search of Metal Nanocatalysts for Oxygen Reduction", **AIChE Annual Meeting**, Pittsburgh, PA, 11/2018
35. **Z. Li***, and H. Xin, "Large-Scale Exploration of Perovskites for Oxygen Evolution Via Adaptive Machine Learning", **AIChE Annual Meeting**, Pittsburgh, PA, 11/2018
34. **H. Xin***, "Machine (& Human!) Learning in Catalyst Discovery", **XXVII International Materials Research Congress,** Cancun, Mexico, 8/2018
33. **H. Xin***, "Overcoming Site Heterogenity in Search of Metal Nanocatalysts for Oxygen Reduction", **XXVII International Materials Research Congress,** Cancun, Mexico, 8/2018
32. **S. Wang***, and H. Xin, "Overcoming Site Heterogeneity in Search of Metal Nanocatalysts for Oxygen Reduction", **ACS Fall Meeting**, Boston, MA, 8/2018
31. **H. Xin***, "Machine Learning Strategies for Accelerating Discovery of Perovskite Electrocatalysts", **Machine Learning in Science/Engineering Conference,** Pittsburgh, PA, 6/2018
30. Z. Li, S. Wang, and **H. Xin***, "Machine (& Human!) Learning in Catalyst Discovery", **ACS Spring Meeting**, New Orleans, LA, 3/2018
29. **H. Xin***, "Data Science in Catalyst Discovery", **guest lecture in Multi-scale Modeling of Materials** (invited by Prof. Sanket A. Deshmukh) at Department of Chemical Engineering at Virginia Tech, Blacksburg, VA, 4/2018
28. J. Wang, and **H. Xin***, "Nonadiabatic Oxygen Activation on Ru(0001) Probed by Machine Learning Molecular Dynamics", **ACS Fall Meeting**, New Orleans, LA, 3/2018
27. S. Wang, and **H. Xin***, "Orbitalwise Coordination Numbers as New Descriptors for Oxygen Reduction Catalyst Design", **ACS Fall Meeting**, New Orleans, LA, 3/2018

26. **H. Xin***, "Empirical Rules, Descriptors, and Learning Algorithms for Catalyst Discovery", **guest lecture in Advanced Inorganic Chemistry** (invited by Prof. Feng Lin) at Department of Chemistry at Virginia Tech, Blacksburg, VA, 12/2017
25. **H. Xin***, "Machine Learning Meets Quantum Chemistry: Using Chemisorption Theory, Algorithms, and Data to Design Electrocatalysts", **departmental seminar at Southern Illinois University**, Carbondale, IL, 12/2017
24. Z. Li, S. Wang, and **H. Xin***, "(**Keynote**) Machine (& Human!) Learning in Catalyst Discovery", the $\mathbf{18}^{th}$ **Chinese National Congress on Catalysis**, Tianjin, China, 10/2017
23. **H. Xin***, "Machine Learning Meets Quantum Chemistry: Using Chemisorption Theory, Algorithms, and Data to Design Electrocatalysts", **departmental seminar at Kunming University of Science and Technology**, Kunming, China, 10/2017
22. **H. Xin***, "Machine Learning Meets Quantum Chemistry: Using Chemisorption Theory, Algorithms, and Data to Design Electrocatalysts", **departmental seminar at chemical engineering at University of Pittsburgh**, Pittsburgh, PA, 9/2017
21. Z. Li, S. Wang, and **H. Xin***, "Machine (& Human!) Learning in Catalyst Discovery", **ACS Fall Meeting**, Washington DC, 8/2017
20. S. Wang, and **H. Xin***, "Orbitalwise Descriptors for Engineering Catalytic Sites Toward (Beyond?) Volcano Limits", **ACS Fall Meeting**, Washington DC, 8/2017
19. 'S. Wang, and **H. Xin***, '(**Keynote**) Orbitalwise Coordination Number as a Reactivity Descriptor for Metal Nanocatalysts", **ACS Spring Meeting**, San Francisco, CA, 4/2017
18. Z. Li, S. Wang, W. Chin, L. Achenie, and **H. Xin***, "Machine (& Human!) Learning in Catalyst Discovery", **ACS Spring Meeting**, San Francisco, CA, 4/2017
17. S. Wang, and **H. Xin***, "Engineering Metal/SnO_x Interfaces for Electrochemical CO_2 Reduction", **ACS Spring Meeting**, San Francisco, CA, 4/2017
16. S. Wang, X. Ma, and **H. Xin***, "Orbitalwise Coordination Number as a Reactivity Descriptor for Metal Nanocatalysts", **AIChE Annual Meeting**, San Francisco, CA, 11/2016
15. **H. Xin***, "A Machine Learning Approach to Catalyst Discovery", **Department of Chemical Engineering at North Carolina State University**, Raleigh, NC, 11/2016
14. **H. Xin***, "Materials Discovery through Computation", **Engineering Research Seminar** to first-year engineering students organized by the Center for the Enhancement of Engineering Diversity (CEED), Blacksburg, VA, 10/2016
13. **H. Xin***, "A Machine Learning Approach to Catalyst Discovery", **Department of Chemical Engineering at Tsinghua University**, Beijing, China, 7/2016
12. **H. Xin***, "A Machine Learning Approach to Catalyst Discovery", **Department of Chemical Engineering at Tianjin University**, Tianjin, China, 7/2016
11. Z. Li, S. Wang, L. Achenie, and **H. Xin***, "Developing a Machine Learning Approach to Catalyst Discovery", the $\mathbf{16}^{th}$ **International Congress on Catalysis**, Beijing, China, 7/2016
10. S. Wang, X. Ma, and **H. Xin***, "Orbitalwise Coordination Number as a Reactivity Descriptor for Metal Nanocatalysts", **ACS Spring Meeting**, San Diego, CA, 4/2016
9. Z. Li, X. Ma, and **H. Xin***,"Generalized Catalyst Design Approach with Linear Scaling Relationships and Machine Learning of Ab-Initio Adsorption Energies", **AIChE Annual Meeting**, Salt Lake City, UT, 11/2015
8. X. Ma, and **H. Xin***, "Design of 100-Terminated Bimetallic Electrocatalysts for CO_2 Reduction to C_2 Species", **AIChE Annual Meeting**, Salt Lake City, UT, 11/2015
7. **H. Xin***, "CO_2 Electrocatalyst Design using a Hybrid Machine Learning and DFT Approach", $\mathbf{25}^{th}$ **North American Catalysis Society Meeting**, Pittsburgh, PA, 6/2015

6. **H. Xin***, "Catalyzing Energy Transformation with High Performance Computing", **High Performance Computing Day**, Virginia Tech, Blacksburg, VA, 4/2015
5. **H. Xin***, "Systematic Identification of Multimetallic Catalysts for Electrochemical CO_2 Reduction using Quantum Chemical Modeling and Machine Learning", **Annual Symposium of The Catalysis Society of Metropolitan New York**, Newark, NJ, 3/2015
4. **H. Xin**, A. Vojvodic, J. Voss, and J. K. Nørskov, and F. Abild-Pedersen*, "Effects of d-Band Shape on the Surface Reactivity of Transition-Metal Alloys", **AIChE Annual Meeting**, Atlanta, GA, 11/2014
3. **H. Xin**, J. LaRue, H. Öberg, J. K., Nørskov, A. Nilsson, and F. Abild-Pedersen*, "Role of Adsorbate-Adsorbate Interactions in Dynamics of Surface Bond Breaking", **AIChE Annual Meeting**, Atlanta, GA, 11/2014
2. **H. Xin***, "Towards Understanding the Surface Reactivity of Transition Metal Catalysts", **National ACS Meeting** in honor of Suljo Linic's ACS Catalysis Lectureship, San Francisco, CA, 8/2014
1. **H. Xin***, "Towards Control of Energetics and Dynamics of Molecule-Surface Interactions in Catalysis", **Department of Chemical Engineering at Virginia Tech**, Blacksburg, VA, 2/2014

Research Group at Virginia Tech

Current Members (6 PhD students, 4 undergraduates, 1 high school student)

- Noushin Omidvar (PhD student, Aug. 2016 -)
- Hemanth Pillai (PhD student, Aug. 2017 -)
- Shih-Han Wang (co-advised PhD student with Prof. Achenie, Aug. 2017 -)
- Tianyou Mou (PhD student, Aug. 2018 -)
- Yang Huang (PhD student, Aug. 2019 -)
- Liping Liu (PhD student, Aug. 2019 -)
- Andy Athawale (Undergraduate student, Mar. 2019 -)
- Nich Goldstein (High school senior, Oct. 2020 -)
- Sam Lightfoot (Undergraduate student, Aug. 2021 -)
- Skandan Chandrasekar (Undergraduate Internship, UWaterloo, Oct. 2021 -)

Previous Members (2 postdoc, 3 PhD, 2 MS students, and 7 undergraduates)

- Xianfeng Ma (Postdoc, Jan. 2015 - Dec. 2016), The University of Tennessee, Knoxville
- Ishan Jain (MS, Aug. 2015 - Nov. 2015), AECOM
- Natalie Chen (BS, Jun. 2015 - Oct. 2016), Honeywell UOP
- Wei Shan Chin (MS, Aug. 2016-July 2017), University of Maryland at Baltimore
- Liang Yu (Postdoc, May 2017 - Mar. 2018), Dalian Institute of Chemical Physics
- Siwen Wang (PhD, Aug. 2015 - May 2020), Toyota Research Institute, Ann Arbor, MI
- Jiamin Wang (PhD, Aug. 2015 - Dec. 2019), TSMC, San Jose
- Zheng Li (PhD, Jan. 2015 - Dec. 2019), Vanguard, Pennsylvania
- Junwei Luo (BS, Feb. 2017 - Aug. 2019), UCLA
- Bryan Ngo (BS, Sep. 2017 - Mar. 2019), VT
- Esther Robb (BS, Nov. 2016 - Nov. 2018), VT
- Emily Marx (BS, May 2017 - Jan. 2020), VT
- Qingmin Mu (BS, Jan. 2020 - Aug. 2021), Caltech
- Sichen Liang (BS, Aug. 2020 - Aug. 2021), VT

Awards for Group Students and Postdocs

- **Siwen Wang**, the Sigma Xi Ph.D. Research Award, 4/2020
- **Jiamin Wang**, the **best student poster award** in Chemical Engineering graduate student annual symposium, Virginia Tech, VA, 4/2019
- **Siwen Wang**, the **3rd place of student presentation award** in Chemical Engineering graduate student annual symposium, Virginia Tech, VA, 4/2019
- **Noushin Omidvar**, the **honorable mention poster award** in SECS 2019 annual symposium, Knoxville, TN, 9/2019
- **Zheng Li**, the **Travel Award** to present at the AIChE Catalysis and Reaction Engineering Division, Orlando, FL, 8/2019.
- **Hemanth Pillai**, the **best student poster award** in SECS 2018 annual symposium, George Tech, GA, 9/2018
- **Siwen Wang**, the **Travel Award** to present at the AIChE Catalysis and Reaction Engineering Division, Pittsburgh, PA, 8/2018.
- **Jiamin Wang**, the **NSF travel award** to present at the CMU-Georgia Tech Symposium on Machine Learning in Science and Engineering, Pittsburgh, PA, 6/2018.
- **Siwen Wang**, the **NSF travel award** to attend the World Congress of Chemical Engineering, Barcelona, Spain, 10/2017.
- **Jiamin Wang**, the **poster award** at the SUNCAT Summer Institute, Stanford University, CA, 8/2017.
- **Siwen Wang**, the **Kokes travel award** at the NAM25, Denver, CO, 6/2017.
- **Zheng Li**, the **Travel Award** to present at the 252nd ACS Annual Meeting, Philadelphia, PA, 8/2016.
- **Zheng Li**, the second place for **student talk competition** in SECS 2016 annual symposium, Clemson University, SC, 9/2016
- **Siwen Wang**, the second place for **student poster competition** in SECS 2016 annual symposium, Clemson University, SC, 9/2016

Professional Services

Journal Editorial

2021 **Guest Editor**, *J. Phys. Energy.*, Issue on machine learning for catalysis and energy storage.

Conference Service

2021 **Co-organizer/Chair for the technical symposium: "Accelerating Catalysis Research with Machine Learning"**, *ACS*, Atlanta.

2021 **Co-organizer/Chair for the technical symposium: "Computational Design of Materials and Systems for Energy Applications"**, *IUPAC/CCCE*, World Congress of Chemistry, Montreal, Canada.

2019 **Vice President of the Southeastern Catalysis Society**.

2017–2019 **Secretary of the Southeastern Catalysis Society**.

2019 **Chair for technical session: "Data Science in Catalysis"**, *NAM26*, Chicago.

2019 **Co-organizer/Chair for technical session: "Data Science in Catalysis"**, *ACS*, Orlando.

2018 **Poster judge of Southeastern Catalysis Society (SECS) Annual Meeting**, Atlanta.

2018 **Organizer/Chair for technical session: "Machine Learning for Catalysis Research"**, *ACS*, New Orleans.

2017 **Co-chair for technical poster session: "Catalysis and Reaction Engineering Division"**, *AIChE*, Minneapolis.

2016 **Chair for technical session: "Computational Catalysis"**, *AIChE*, San Francisco.

2016 **Chair for technical session: "Computational Chemistry for Energy Applications"**, *ACS*, Philadelphia.

2016 **Chair for technical session: "Computational Chemistry for Energy Applications"**, *ACS*, San Diego.

2015 **Co-chair for technical session: "Computational Catalysis"**, *AIChE*, Salt Lake City.

2014 **Co-chair for technical session: "Computational Catalysis"**, *AIChE*, Atlanta.

2014 **Poster judge of Southeastern Catalysis Society (SECS) Annual Meeting**, Asheville.

2012 **Co-chair for technical session: "Fundamental Surface Reactivity"**, *AIChE*, Pittsburgh.

Department/College/University Service

2021 **Department Head Search Committee**.

2018 **CHE Rep to the AIChE Recruitment Fair**.

2017 **Faculty Search Committee**.

2015 **Faculty Search Committee**.

2014 **Graduate Recruitment Committee**.

2014 **University Commencement Asst. Marshal**.

Teaching

- "**Data Analytics in Chemical Engineering**", Virginia Tech, Spring 2022
- "**Data Science for Chemical Engineers**", Virginia Tech, Spring 2019/2020
- "**ChE Simulations**", Virginia Tech, Spring 2016/2017/2018/2021, Fall 2021
- "**Computational Catalysis**", Virginia Tech, Fall 2016
- "**Advanced Thermodynamics**", Virginia Tech, Fall 2014/2015/2018/2019/2020
- "**Fundamental Catalysis**", Stanford University, Spring 2014
- "**ChE Unit Operation**", University of Michigan, Ann Arbor, Spring 2010

Review Service

- **Proposals**: NSF, ACS PRF, AFSOR, DoE, ARO
- **Journals**: 20+ journals including Science, Nature Chemistry, ACS Catalysis, Journal of Physical Chemistry Letters, JACS, Surface Science, Journal of Chemical Physics, Langmuir, Journal of Physical Chemistry A, Journal of Physical Chemistry C, Scientific Reports, Chemistry of Materials, Industrial & Engineering Chemistry Research, Environmental Science: Processes & Impacts, Catalysis Today, Calphad, Applied Catalysis A: General, RSC Advances, Journal of Materials Chemistry A., Reaction Chemistry & Engineering, Applied Catalysis B: Environmental, Catalysis Science & Technology, Nature Catalysis, Advanced Energy Materials, NPJ Computational Materials, Nano Energy, Catalysis Today

Memberships

- American Institute of Chemical Engineers (AIChE)
- American Chemical Society (ACS)
- North American Catalysis Society (NACS)
- Southeastern Catalysis Society (SECS)