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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

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

2025 **Professor**, *Chemical Engineering, Virginia Tech*

2020–2025 **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

- Energy, Sustainability, Climate Solutions, Circular Economy
- Artificial Intelligence (AI), Quantum Chemistry, Multiscale Simulations
- Electronic Structure Theory, Catalysis Theory, Statistical Learning Theory
- Heterogeneous Catalysis, Electrocatalysis, Plasmonic Photochemistry

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 16th 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*

Invited Lectures and Presentations

93. **H. Xin***, "Agentic Artificial Intelligence (AI) for Accelerating Catalytic Materials Research", **NAM 29**, Atlanta, GA, 06/2025
92. **H. Xin***, "AI for Multidisciplinary Exploration and Discovery (AIMED) Workshop on Heterogeneous Catalysis: A Report", **DOE BES/Catalysis Science PI Meeting**, MD, 11/2024
91. **H. Xin***, "Artificial Intelligence for Accelerating Catalytic Materials Discovery", **DOE BES/Catalysis Science PI Meeting**, MD, 11/2024
90. **H. Xin***, "Emergence of Agentic AI for Accelerating Catalytic Materials Research", **EICARPA-E AI Workshop**, Virtual, 9/2024
89. **H. Xin***, "Accelerating Catalytic Materials Discovery with Artificial Intelligence", **ACS Fall Meeting**, Denver, CO, 8/2023
88. **H. Xin***, "Unifying Theory of Electronic Descriptors of Metal Surfaces upon Perturbation", **ACS Fall Meeting**, Denver, CO, 8/2023
87. **H. Xin***, "Advancing Catalysis Theory with Theory-infused Deep Learning", **ACS Fall Meeting**, Denver, CO, 8/2023
86. **H. Xin***, "Accelerating Scientific Discovery in Catalysis with Artificial Intelligence", **AIMS Workshop**, NIST, Gaithersburg, MD, 7/2024
85. **H. Xin***, "Accelerating Catalytic Materials Discovery toward Sustainability with Artificial Intelligence", **Materials Science and Engineering**, Virginia Tech, VA, 4/2024
84. **H. Xin***, "Accelerating Materials Discovery toward a Sustainable Future with Artificial Intelligence", **MACR 5016**, Virginia Tech, VA, 4/2024
83. **H. Xin***, "AI-powered Catalytic Materials Discovery toward Sustainability", **ACS Spring Meeting**, New Orleans, LA, 3/2023
82. **H. Xin***, "Interpretable Machine Learning of Interfacial Electrokinetics of Hydrogen Evolution", **ACS Spring Meeting**, New Orleans, LA, 3/2023
81. **H. Xin***, "Interpretable Machine Learning for Accelerating Catalytic Materials Design toward Sustainable Ammonia Chemistry", **ACS Spring Meeting**, New Orleans, LA, 3/2023
80. **H. Xin***, "Advancing Catalysis Science for Sustainability with Artificial Intelligence", **Chemistry and Chemical Engineering Division Seminar**, Southwest Research Institute, San Antonio, TX, 2/2024
79. **H. Xin***, "Advancing Catalysis Science for Sustainability with Artificial Intelligence", **Chemistry Division Seminar**, Naval Surface Warfare Center, Indian Head, MD, 1/2024
78. **H. Xin***, "Accelerating Scientific Discovery in Catalysis with Artificial Intelligence", **Chemistry Division Seminar**, Brookhaven National Laboratory, NY, 11/2023

77. **H. Xin***, "Advancing Scientific Discovery in Catalysis with Artificial Intelligence", **Energy Seminar at UCF**, Orlando, FL, 11/2023
76. **H. Xin***, "From Alchemy to AI: Engineering Materials toward Sustainability", **Virginia Society of Professional Engineers (VSPE) meeting**, Blacksburg, VA, 10/2023
75. **H. Xin***, "From Alchemy to AI: Harnessing the Power of Data for Catalytic Materials Design", **Chemical and Life Science Engineering Seminar at VCU**, Richmond, VA, 10/2023
74. **H. Xin***, "From Alchemy to AI: Harnessing the Power of Data for Catalytic Materials Design", **Chemistry Seminar at Iowa State University**, Ames, IA, 10/2023
73. **H. Xin***, "Catalytic Materials Design toward Sustainability with Interpretable Deep Learning", **Physical Chemistry Seminar at University of Florida**, Gainesville, FL, 9/2023
72. **H. Xin***, "Machine Learning for Accelerating Catalytic Materials Discovery", **Chemical Engineering Seminar at UMass Lowell**, Lowell, MA, 9/2023
71. **H. Xin***, "Sustainable Ammonia Electrocatalysis with Theory-guided Design of Multimetallic Nanostructures", **ACS Fall Meeting**, San Francisco, 08/2023
70. **H. Xin***, "Interpretable Deep Learning for Predicting Electronic Descriptors of Metal Surfaces upon Perturbation", **ACS Fall Meeting**, San Francisco, 08/2023
69. **H. Xin***, "Advancing Catalysis Theory and Materials Design with Machine Learning", **ACS Fall Meeting**, in honor of S. Ted Oyama for the George A. Olah Award, San Francisco, 08/2023
68. **H. Xin***, "Catalytic Materials Design toward Sustainability with Machine Learning", **Virginia Clean Energy and Catalysis Summit**, Richmond, 08/2023
67. **H. Xin***, "Interpretable Design of Ir-free Trimetallic Electrocatalysts for Ammonia Oxidation with Graph Neural Networks", **CSC Meeting**, Vancouver, 06/2023
66. **H. Xin***, "Breaking Linear Adsorption-Energy Scaling Limitations of Electrocatalytic NO_3^- Reduction via Machine-Learned Insights", **ACS Spring Meeting**, Indianapolis, 03/2023
65. **H. Xin***, "Breaking Linear Adsorption-Energy Scaling Limitations of Electrocatalytic NO_3^- Reduction via Machine-Learned Insights", **ACS Spring Meeting**, Indianapolis, 03/2023
64. **H. Xin***, "Discovery of Pt Trimetallic Electrocatalysts for Ammonia Oxidation with Interpretable Deep Learning", **ACS Spring Meeting**, Indianapolis, 03/2023
63. **H. Xin***, "Advancing Theory of Chemical Bonding at Surfaces with Machine Learning", **ACS Spring Meeting**, in honor of Suljo Linic for the Gabor A. Somorjai Award, Indianapolis, 03/2023
62. **H. Xin***, "Advancing Theory of Interfacial Catalysis with Machine Learning", **departmental seminar in the Department of Chemistry at Boston College**, Chestnut Hill, MA, 10/2022
61. **H. Xin***, "Interpretable Machine Learning for Catalysis beyond Energy Scaling Limitations", **ACS Fall Meeting**, in honor of Eranda Nikolla for 2022 ACS Catalysis Lectureship, Chicago, 08/2022
60. **H. Xin***, "Interpretable Deep Learning Reveals the Catalyst Genome for Oxygen Reduction ", **ACS Fall Meeting**, Chicago, 08/2022
59. **H. Xin***, "Accelerating Multimetallic Catalysts Discovery for Ammonia Electrooxidation via Interpretable Deep Learning", **ACS Fall Meeting**, Chicago, 08/2022
58. **H. Xin***, "Interpretable Machine Learning for Accelerating Catalytic Materials Discovery", **Gordon Catalysis**, New London, NH, 6/2022
57. **H. Xin***, "Advancing Catalytic Materials Discovery and Theoretical Knowledge with Interpretable Machine Learning", **27th NAM Meeting**, New York City, NY, 5/2022
56. **H. Xin***, "Three Facets of Interpretable Machine Learning for Advancing Catalysis Theory and Catalytic Materials Discovery", **Catalysis Club of Chicago Spring Symposium**, Chicago, IL, 5/2022

55. **H. Xin***, "Advancing Catalytic Materials for Ammonia Redox Cycling by Machine Learning", **Catalysis Club of Philadelphia (CCP)**, Virtual, 4/2022
54. **H. Xin***, "Artificial Intelligence for Accelerating Catalytic Materials Discovery", **AI Materials Workshop**, Virginia Tech, 4/2022
53. **H. Xin***, "Interpretable Machine Learning for Accelerating Catalytic Materials Discovery", **the Canadian Chemical Engineering Conference (CCEC)**, Virtual, 10/2021
52. **H. Xin***, "Interpretable Machine Learning for Accelerating Catalytic Materials Discovery", **SUNCAT ML Workshop**, Virtual, 09/2021
51. **H. Xin***, "Bayesian Learning Reveals the Nature of Chemical Bonding at Single Atom Alloys", **ACS Fall Meeting**, in honor of Phil Christopher for CATL Early Career Award, Atlanta, 08/2021
50. Hemanth S. Pillai, Siwen Wang, and **H. Xin***, "Interpretable Machine Learning of Chemical Bonding at Solid Surfaces", **ACS Fall Meeting**, Atlanta, 08/2021
49. **H. Xin***, "Theory-Infused Machine Learning of Chemisorption at Metal Surfaces", **IUPAC CCCE**, Virtual, 08/2021
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", **The Minerals, Metals & Materials Society (TMS) Meeting**, 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 **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 **16th 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", **25th 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

Publications at Virginia Tech (Google Citations: >11350, h-index: 39)

80 C. Kuai, L. Liu, A. Hu, Y. Zhang, Y. Zhang, D. Xia, D. Nordlund, D. Sokaras, D. Decarolis, D. Gianolio, **H. Xin***, L. Liu*, and F. Lin* (May 2025). "Dissolved Fe species enable a cooperative solid–molecular mechanism for the oxygen evolution reaction on NiFe-based catalysts". In: **Nat. Catal.** Pp. 1–13. *doi: 10.1038/s41929-025-01342-5*.

79 Z. Zhang, E. Hershkovitz, Q. An, L. Liu, X. Wang, Z. Deng, G. Baucom, W. Wang, J. Zhao, Z. Xin, L. Moore, Y. Yao, M. R. U. Islam, X. Chen, B. Cui, L. Li, **H. Xin**, L. Li, H. Kim, and W. Cai* (Nov. 2024). "Spinel oxide enables high-temperature self-lubrication in superalloys". In: **Nat. Commun.** 15.1, p. 10039. *doi: 10.1038/s41467-024-54482-w*.

78 Y. Huang, S.-H. Wang, L. E. K. Achenie, K. Choudhary, and **H. Xin*** (Oct. 2024). "Origin of unique electronic structures of single-atom alloys unraveled by interpretable deep learning". In: **J. Chem. Phys.** 161.

77 Y. Huang, S.-H. Wang, M. Kamnuru, L. E. Achenie, J. R. Kitchin*, and **H. Xin*** (Sept. 2024). "Unifying theory of electronic descriptors of metal surfaces upon perturbation". In: **Phys. Rev. B** 110.12, p. L121404. *doi: 10.1103/PhysRevB.110.L121404*.

76 S. Xie, L. Liu, Y. Li, K. Ye, D. Kim, X. Zhang, **H. Xin***, L. Ma, S. N. Ehrlich, and F. Liu* (Sept. 2024). "Zeolite-promoted platinum catalyst for efficient reduction of nitrogen oxides with hydrogen". In: **Nat. Commun.** 15.1, pp. 1–11. *doi: 10.1038/s41467-024-52382-7*.

75 L. Liu, Q. Xu, L. Dos Anjos Cunha, **H. Xin**, M. Head-Gordon, and J. Qian* (July 2024). "Real-space pseudopotential method for the calculation of third-row elements X-ray photoelectron spectroscopic signatures". In: **J. Chem. Theory Comput.** 20.14, pp. 6134–6143. *doi: 10.1021/acs.jctc.4c00535*.

74 Y. Huang, S.-H. Wang, X. Wang, N. Omidvar, L. E. K. Achenie, S. E. Skrabalak, and **H. Xin*** (July 2024). "Unraveling reactivity origin of oxygen reduction at high-entropy alloy electrocatalysts with a computational and data-driven approach". In: **J. Phys. Chem. C Nanomater. Interfaces** 128.27, pp. 11183–11189. *doi: 10.1021/acs.jpcc.4c01630*.

73 D. K. Choudhary*, K. Li, K. F. Garrity, V. Gupta, A. H. Romero, J. T. Krogel, K. Saritas, A. Fuhr, P. Ganesh, P. R. C. Kent, K. Yan, Y. Lin, S. Ji, B. Blaiszik, P. Reiser, P. Friederich, A. Agrawal, P. Tiwary, E. Beyerle, P. Minch, T. D. Rhone, I. Takeuchi, R. B. Wexler, A. Mannodi-Kanakkithodi, E. Ertekin, A. Mishra, N. Mathew, M. Wood, A. D. Rohskopf, J. Hattrick-Simpers, S.-H. Wang, L. E. K. Achenie, **H. Xin**, M. Williams, A. J. Biacchi, and F. Tavazza (May 2024). "JARVIS-Leaderboard: a large scale benchmark of materials design methods". In: **npj Computational Materials** 10.1, pp. 1–17. *doi: 10.1038/s41524-024-01259-w*.

72 N. Omidvar, S.-H. Wang, Y. Huang, H. S. Pillai, A. Athawale, S. Wang, L. E. K. Achenie, and **H. Xin*** (Mar. 2024). "Explainable AI for optimizing oxygen reduction on Pt monolayer core–shell catalysts". In: **Electrochem. Sci. Adv.** e202300028. *doi: 10.1002/elsa.202300028*.

71 L. Liu, C. B. Thompson, T. Mou, A. Karim*, and **H. Xin*** (Jan. 2024). "Elucidation of site structures and CO oxidation kinetics of the Ir_1/TiO_2 single-atom catalyst". In: **Chem Catalysis**, p. 100900. *doi: 10.1016/j.checat.2024.100900*.

70 S. Wang, L. Liu, **H. Xin***, and C. Ling* (Jan. 2024). "Toward a stable and active catalyst for proton-exchange membrane water electrolysis". In: **Chem Catalysis** 4.1, p. 100869. *doi: 10.1016/j.checat.2023.100869*.

69 L. Liu, S. Wang, C. Ling*, and **H. Xin*** (Jan. 2024). "Advancing oxygen evolution electrocatalysis with human-machine intelligence". In: **Chem Catalysis** 4.1, p. 100868. *doi: 10.1016/j.checat.2023.100868*.

68 R. Perez, Y. Huang, H. S. Pillai, and **H. Xin*** (Dec. 2023). "Recent Advances and Fundamental Challenges in Computational Modeling of Electrocatalytic Ammonia Oxidation". In: **ACS EST Eng.** *doi: 10.1021/acsestengg.3c00415*.

67 **H. Xin***, T. Mou, H. Pillai, S.-H. Wang, and Y. Huang (2024). "Interpretable Machine Learning for Catalytic Materials Design toward Sustainability". In: **Acc. Mater. Res.** *doi: 10.1021/accountsmr.3c00131*.

66 J. Chen, Z. Zhang, E. Hershkovitz, J. Poplawsky, R. S. B. Dandu, C.-Y. Hung, W. Wang, Y. Yao, L. Li*, **H. Xin**, H. Kim*, and W. Cai* (Jan. 2024). "Selective oxidation and nickel enrichment hinders the repassivation kinetics of multi-principal element alloy surfaces". In: **Acta Mater.** 263, p. 119490. *doi: 10.1016/j.actamat.2023.119490*.

65 M. S. Hossain, G. S. Dhillon, L. Liu, A. Sridhar, E. J. Hiennadi, J. Hong, S. R. Bare, **H. Xin**, T. Ericson, A. Cozzolino, and S. Khatib* (Nov. 2023). "Elucidating the role of Fe-Mo interactions in the metal oxide precursors for Fe promoted Mo/ZSM-5 catalysts in non-oxidative methane dehydroaromatization". In: **Chem. Eng. J.** 475, p. 146096. *doi: 10.1016/j.cej.2023.146096*.

64 Q. Gao, Z. Yan, W. Zhang, H. S. Pillai, B. Yao, W. Zang, Y. Liu, X. Han, B. Min, H. Zhou, L. Ma, B. Anaclet, S. Zhang, **H. Xin***, Q. He*, and H. Zhu* (Aug. 2023). "Atomic Layers of B2 CuPd on Cu Nanocubes as Catalysts for Selective Hydrogenation". In: **J. Am. Chem. Soc.** *doi: 10.1021/jacs.3c06514*.

63 X. Wang, Y. Huang, X. Xie, Y. Liu, Z. Huo, M. Lin, **H. Xin***, and R. Tong* (June 2023). "Bayesian-optimization-assisted discovery of stereoselective aluminum complexes for ring-opening polymerization of racemic lactide". In: **Nat. Commun.** 14.1, pp. 1–11. *doi: 10.1038/s41467-023-39405-5*.

62 C. B. Thompson, L. Liu, D. S. Leshchev, A. S. Hoffman, J. Hong, S. R. Bare, R. R. Unocic, E. Stavitski, **H. Xin***, and A. Karim* (May 2023). "CO Oxidation on Ir_1/TiO_2: Resolving Ligand Dynamics and Elementary Reaction Steps". In: **ACS Catal.** Pp. 7802–7811. *doi: 10.1021/acscatal.3c01433*.

61 Q. Gao, B. Yao, H. Pillai, W. Zang, X. Han, Y. Liu, S.-W. Yu, Z. Y. Yan, B. Min, S. Zhang, H. Zhou, L. Ma, **H. Xin***, Q. He*, and H. Zhu* (Mar. 2023). "Synthesis of core/shell nanocrystals with ordered intermetallic single-atom alloy layers for nitrate electroreduction to ammonia". In: **Nat. Synth.** Pp. 1–11. *doi: 10.1038/s44160-023-00258-x*.

60 T. Mou, H. S. Pillai, S. Wang, M. Wan, X. Han, N. M. Schweitzer, F. Che, and **H. Xin*** (Feb. 2023). "Bridging the complexity gap in computational heterogeneous catalysis with machine learning". In: **Nat. Catal** 6.2, pp. 122–136. *doi: 10.1038/s41929-023-00911-w*.

59 H. S. Pillai, Y. Li*, S.-H. Wang, N. Omidvar, Q. Mu, L. E. K. Achenie, F. Abild-Pedersen, J. Yang, G. Wu*, and **H. Xin*** (Feb. 2023). "Interpretable design of Ir-free trimetallic electrocatalysts for ammonia oxidation with graph neural networks". In: **Nat. Commun.** 14.1, pp. 1–11. *doi: 10.1038/s41467-023-36322-5*.

58 S. Xie, L. Liu, Y. Lu*, C. Wang, S. Cao, W. Diao, J. Deng, W. Tan, L. Ma, S. Ehrlich, Y. Li, Y. Zhang, K. Ye, **H. Xin***, M. Flytzani-Stephanopoulos, and F. Liu* (Nov. 2022). "Pt Atomic Single-Layer Catalyst Embedded in Defect-Enriched Ceria for Efficient CO Oxidation". In: **J. Am. Chem. Soc.** *doi: 10.1021/jacs.2c08902*.

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56 Z. Zhang, Y. Yao, L. Liu, T. Mou, **H. Xin***, L. Li, and W. Cai* (Aug. 2022). "Computational design of non-equiatomic CoCrFeNi alloys towards optimized mechanical and surface properties". In: **J. Mater. Res.** *doi: 10.1557/s43578-022-00695-y*.

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Research Group at Virginia Tech

Current Members (5 PhD students, 1 MS student)

- Shih-Han Wang (co-advised PhD student with Prof. Achenie, Aug. 2017 -)
- Liping Liu (PhD student, Aug. 2019 -)
- Xiangrui Wang (PhD student, Aug. 2021 -)
- Shuyi Cao (PhD student, Aug. 2024 -)
- Raul Diaz Aquino (PhD student, Aug. 2023 -)

Previous Members (2 postdocs, 7 PhD students, 2 MS students, 11 undergraduates, and 1 high schooler)

- 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
- Nich Goldstein (High school senior, Oct. 2020 Jan. 2021)
- Skandan Chandrasekar (Undergraduate Internship, UWaterloo, Oct. 2021 - Jan. 2022)
- Noushin Omidvar (PhD, Aug. 2016 - Sept. 2022), VT
- Hemanth S. Pillai (PhD, Aug. 2017 - Dec. 2022), postdoc at the Theory Department - Fritz Haber Institute
- Andy Athawale (Undergraduate student, Mar. 2019 - Jan. 2023)
- Sam Lightfoot (Undergraduate student, Aug. 2021 - Jan. 2023)
- Tianyou Mou (PhD, Aug. 2018 - Jun. 2023), postdoc at the Brookhaven National Lab
- Yang Huang (PhD student, Aug. 2019 - Jun. 2024), postdoc at Dartmouth College

Awards for Group Students and Postdocs

- **Liping Liu**, the **Travel Award** to present at the AIChE Catalysis and Reaction Engineering Division, San Diego, CA, 11/2024
- **Liping Liu**, the **CATL-ChemCatBio Graduate Student Travel Award** for presenting at the ACS 2023 Fall meeting, San Francisco, CA, 8/2023
- **Yang Huang**, the **CATL-ChemCatBio Graduate Student Travel Award** for presenting at the ACS 2023 Fall meeting, San Francisco, CA, 8/2023
- **Tianyou Mou**, the **2023 Kokes Award** for the 28th North American Catalysis Society meeting, Providence, RI, 6/2023
- **Hemanth Pillai**, the **Travel Award** to present at the AIChE Catalysis and Reaction Engineering Division, Phoenix, AZ, 11/2022
- **Hemanth Pillai**, the **best poster presentation award** at the Virginia Clean Energy and Catalysis Summit, Charlottesville, VA, 8/2022
- **Hemanth Pillai**, the **best oral presentation award** at the Southeastern Catalysis Society meeting, Atlanta, GA, 2/2022
- **Liping Liu**, the **first place of the poster presentation award** at the Southeastern Catalysis Society meeting, Atlanta, GA, 2/2022
- **Hemanth Pillai**, the **2022 Kokes Award** for the 27th North American Catalysis Society meeting, New York City, NY, 5/2022
- **Hemanth Pillai**, the **travel award** for presenting at the ACS 2021 Fall meeting, Atlanta, GA, 9/2021
- **Siwen Wang**, the **Sigma Xi Ph.D. Research Award**, Sigma Xi VT Chapter, 4/2020
- **Jiamin Wang**, the **best student poster award** in Chemical Engineering graduate student annual symposium, Virginia Tech, VA, 4/2019
- **Hemanth Pillai**, the **NSF non-academic research internship award**, SLAC national lab, 9/2019 - 1/2020
- **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
- **Hemanth Pillai**, the **2nd place of the Data Science Competition Award**, Virginia Tech ChE, 5/2019
- **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

2024 **Guest Editor**, *Journal of Chemical Physics*, Special Issue: Machine Learning Methods for Interfacial Catalysis.

2024 **Guest Editor**, *Journal of Catalysis*, Special Issue: Catalytic Materials Discovery in the Age of Data Science.

2023 **Guest Editor**, *Electrochemical Science Advances (ELSA)*, Special Issue: Machine Learning in Electrocatalysis.

2022 **Guest Editor**, *Engineering*, Special Issue: Artificial Intelligence in Chemical Engineering.

2021 **Guest Editor**, *J. Phys. Energy.*, Special Issue: Machine Learning for Catalysis and Energy Materials.

Conference Service

2025 **Communications Director**, *North American Catalysis Society*.

2024 **Inaugural chair for the Artificial Intelligence for Multidisciplinary Exploration and Discovery (AIMED) Workshop in Heterogeneous Catalysis**, *Chicago, IL*.

2023 **Program co-chair for the North American Catalysis Society Meeting**, *NAM*, Atlanta.

2023 **Organizer/Chair for the technical symposium: "Data Science for Catalysis"**, *ACS*, San Francisco.

2023 **Bin Chair for AIChE Topical - Applications of Data Science in Catalysis and Reaction Engineering"**, *AIChE*, Orlando.

2023 **Organizer/Chair for the technical topic: "Modeling, Simulation, and Machine Learning"**, *NAM28*, Providence.

2023 **Past President of the Southeastern Catalysis Society**.

2021 **President of the Southeastern Catalysis Society**.
2023

2022 **Co-chair for AIChE Topical - Applications of Data Science in Catalysis and Reaction Engineering"**, *AIChE*, Phoenix.

2022 **Co-organizer/Chair for AIChE 20A - Data Science & Machine Learning Approaches to Catalysis"**, *AIChE*, Phoenix.

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.

2019–2021 **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

2023 **Chemistry Faculty Search Committee**.

2021 **Department Head Search Committee**.

2019 **Chair of the CHE Data Science 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

- "**Machine Learning in Chemical Sciences and Engineering** ", Virginia Tech, Fall 2022
- "**Explainable AI for Domain Insights**", Virginia Tech, Spring 2023
- "**Data Science for Chemical Engineers**", Virginia Tech, Spring 2019/2020

- "**ChE Simulations**", Virginia Tech, Spring 2016/2017/2018/2021/2022, Fall 2021, Spring 2022
- "**Computational Catalysis**", Virginia Tech, Fall 2016
- "**Advanced Thermodynamics**", Virginia Tech, Fall 2014/2015/2018/2019/2020/2023
- "**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**: 30+ journals including Science, Nature, 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)
- Materials Research Society (MRS)
- Southeastern Catalysis Society (SECS)