

Department of Chemical Engineering, Virginia Tech
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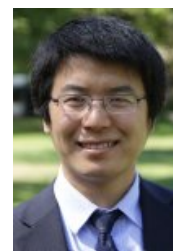
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Hongliang Xin

Curriculum Vitæ

Research Interests

- *Electronic Structure Theory and Methods*
- *Machine Learning and Materials Informatics*
- *Fundamentals of Surface Reactivity*
- *Multiscale Kinetic Modeling of Surface Reactions*
- *Ab-Initio Modeling of Electrochemical Interfaces*
- *Metal-Organic Frameworks (MOFs) for Catalysis and (Photo)electrocatalysis*
- *Photocatalytic Water Splitting on Plasmonic Metal/Metal Oxide Nanoassemblies*
- *Single Atom/Site Catalysis*
- *Fuel Cell Catalysis*
- *Electrochemical CO₂ Reduction and Ammonia Synthesis*
- *Lithium-ion and Metal-air Batteries*

Academic Appointments

2014

Assistant Professor, Virginia Tech, Blacksburg.

2013

Postdoctoral Research Fellow, Stanford University/SLAC.

2014

Research areas: The *d*-band Chemisorption Theory, Dynamic Modeling of Surface Reactions

2011

Postdoctoral Research Fellow, University of Michigan, Ann Arbor.

2013

Research areas: Quantum Chemical Modeling of Electron-driven Reactions, Fuel Cell Catalysis

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 with Perturbed Electronic Properties*

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

Honors & Awards

2017

Journal of Materials Chemistry A - 2017 Emerging Investigators.

2016

NSF Travel Award for Attending 16th International Congress on Catalysis, Beijing, China.

2016

ICTAS Junior Faculty Award, Virginia Tech.

- 2015 ACS 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 Rackham Travel Award, University of Michigan, Ann Arbor, MI.
- 2011
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

- 29 S. Wang, N. Omidvar, E. Marx, and H. Xin* (2017). "Coordination Numbers for Unraveling Intrinsic Size Effects in Gold-catalyzed CO Oxidation". In: **Phys. Chem. Chem. Phys.**, **Accepted**.
- 28 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: <http://dx.doi.org/10.1039/C7TA01812F>.
- 27 S. Wang, J. Wang, and H. Xin* (2017). "Insights into Electrochemical CO₂ Reduction on Tin Oxides from First-principles Calculations". In: **Green Energy & Environment** 2.2, pp. 168–171. doi: <http://dx.doi.org/10.1016/j.gee.2017.02.005>.
- 26 W. Luc, C. Collins, S. Wang, H. Xin, K. He, Y. Kang, and F. Jiao* (2017). "Ag-Sn Bimetallic Catalyst with a Core-Shell Structure for CO₂ Reduction". In: **J. Am. Chem. Soc.** 139.5, pp. 1885–1893. doi: <http://dx.doi.org/10.1021/jacs.6b10435>.
- 25 Z. Li, X. Ma, and H. Xin* (2017). "Feature Engineering of Machine-learning Chemisorption Models for Catalyst Design". In: **Catal. Today** 280, Part 2, pp. 232–238. doi: <https://doi.org/10.1016/j.cattod.2016.04.013>.
- 24 X. Ma and H. Xin* (2017). "Orbitalwise Coordination Number for Predicting Adsorption Properties of Metal Nanocatalysts". In: **Phys. Rev. Lett.** 118.3, p. 036101. doi: <http://dx.doi.org/10.1103/PhysRevLett.118.036101>.
- 23 H. Xin* and S. Lincic* (2016). "Analyzing Relationships between Surface Perturbations and Local Chemical Reactivity of Metal Sites: Alkali Promotion of O₂ Dissociation on Ag(111)". In: **J. Chem. Phys.** 144.23, p. 234704. doi: <http://dx.doi.org/10.1063/1.4953906>.
- 22 X. Ma, Z. Li, L. E. K. Achenie, and H. Xin* (2015). "Machine-Learning-Augmented Chemisorption Model for CO₂ Electroreduction Catalyst Screening". In: **J. Phys. Chem. Lett.** Pp. 3528–3533. doi: <10.1021/acs.jpcllett.5b01660>.
- 21 X. Ma, J. S. A. Carneiro, X.-K. Gu, H. Qin, H. Xin, K. Sun, and E. Nikolla* (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)

- 20 J. LaRue, O. Krejčí, 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 (2017). “Real-Time Elucidation of Catalytic Pathways in CO Hydrogenation on Ru”. In: **J. Phys. Chem. Lett.** 8.16, pp. 3820–3825. doi: <http://dx.doi.org/10.1021/acs.jpcllett.7b01549>.
- 19 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 (2016). “Chemical Bond Activation Observed with an X-ray Laser”. In: **J. Phys. Chem. Lett.** 7.18, pp. 3647–3651.
- 18 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* (2015). “Probing the Transition State Region in Catalytic CO Oxidation on Ru”. In: **Science** 347.6225, pp. 978–982. doi: [10.1126/science.1261747](https://doi.org/10.1126/science.1261747).
- 17 **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* (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](https://doi.org/10.1103/PhysRevLett.114.156101).
- 16 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](https://doi.org/10.1021/nl502571b).
- 15 **H. Xin**, A. Vojvodic, J. Voss, J. K. Nørskov, and F. Abild-Pedersen* (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](https://doi.org/10.1103/PhysRevB.89.115114).
- 14 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](https://doi.org/10.1021/ar3002393).
- 13 A. Holewinski, **H. Xin**, E. Nikolla, and S. Linic* (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](https://doi.org/10.1016/j.coche.2013.04.006).
- 12 P. Christopher, **H. Xin**, A. Marimuthu, and S. Linic* (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](https://doi.org/10.1038/nmat3454).
- 11 **H. Xin**, A. Holewinski, N. Schweitzer, E. Nikolla, and S. Linic* (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](https://doi.org/10.1007/s11244-012-9794-2).
- 10 **H. Xin**, A. Holewinski, and S. Linic* (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](https://doi.org/10.1021/cs200462f).
- 9 P. Christopher, **H. Xin**, and S. Linic* (2011). “Visible-light-enhanced Catalytic Oxidation Reactions on Plasmonic Silver Nanostructures”. In: **Nat Chem** 3.6, pp. 467–472. doi: [10.1038/nchem.1032](https://doi.org/10.1038/nchem.1032).

- 8 **H. Xin** and S. Linic* (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](https://doi.org/10.1063/1.3437609).
- 7 **H. Xin**, N. Schweitzer, E. Nikolla, and S. Linic* (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](https://doi.org/10.1063/1.3336015).
- 6 N. Schweitzer, **H. Xin**, E. Nikolla, J. T. Miller, and S. Linic* (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](https://doi.org/10.1007/s11244-010-9448-1).
- 5 Q. Wu, M.-H. Han*, **H. Xin**, B.-Q. Dong, and Y. Jin (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.
- 4 Q. Wu, B.-Q. Dong, M.-H. Han*, **H. Xin**, Y.-Z. Zuo, and Y. Jin (2007). "Studies on Acidity of Chloroaluminate 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.
- 3 **H. Xin**, Q. Wu, M. Han*, D. Wang, and Y. Jin (2005). "Alkylation of Benzene with 1-dodecene in Ionic Liquids [Rmim]⁺Al₂Cl₆X⁻ (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](https://doi.org/10.1016/j.apcata.2005.06.012).

Invited Lectures and Presentations

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 **18th 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 CO₂ 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 CO₂ Reduction to C₂ Species", **AIChE Annual Meeting**, Salt Lake City, UT, 11/2015
7. **H. Xin***, "CO₂ 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 CO₂ 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 (1 postdoc, 5 PhD students, and 4 undergraduates)

- Liang Yu (Postdoc May 2017 -)
- Zheng Li (PhD student, Jan. 2015 -)
- Siwen Wang (PhD student, Aug. 2015 -)
- Jiamin Wang (PhD student, Aug. 2015 -)
- Noushin Omidvar (PhD student, Aug. 2016 -)
- Hemanth Pillai (PhD student, Aug. 2017 -)
- Esther Robb (Undergraduate student, Nov. 2016 -)

- Junwei Luo (Undergraduate student, Feb. 2017 -)
- Emily Marx (Undergraduate student, May 2017 -)
- Bryan Ngo (Undergraduate student, Sep. 2017 -)

Previous Members (1 postdoc, 2 MS students, and 1 undergraduate)

- Xianfeng Ma (Jan. 2015 - Dec. 2016), The University of Tennessee, Knoxville
- Ishan Jain (Aug. 2015 - Nov. 2015), AECOM
- Natalie Chen (Jun. 2015 - Oct. 2016), Honeywell UOP
- Wei Shan Chin (Aug. 2016-July 2017), University of Maryland at Baltimore

Awards for Group Students and Postdocs

- **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 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

Conference Service

2017 Secretary of the Southeastern Catalysis Society.

2018 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

2017 CHE Rep to the Engineering Faculty Organization (Alternative) .

2017 Faculty Search Committee.

2015 Faculty Search Committee.

2014 Graduate Recruitment Committee.

2014
2017 University Commencement Asst. Marshal.

Teaching

- “**ChE Simulations**”, Virginia Tech, Spring 2017
- “**Elective Course: Computational Catalysis**”, Virginia Tech, Fall 2016
- “**ChE Simulations**”, Virginia Tech, Spring 2016
- “**Advanced Thermodynamics**”, Virginia Tech, Fall 2015
- “**Advanced Thermodynamics**”, Virginia Tech, Fall 2014
- “**TA for Fundamental Catalysis**”, Stanford University, Spring 2014
- “**TA for ChE Unit Operation**”, University of Michigan, Ann Arbor, Spring 2010

Review Service

- **Proposals:** NSF, ACS PRF, AFSOR
- **Journals:** 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

Memberships

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