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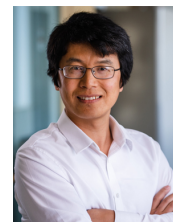
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# Hongliang Xin

## Curriculum Vitæ

### Research Interests

- *Ab Initio Machine Learning*
- *Catalysis Theory and Informatics*
- *Multiscale Modeling of Catalytic Processes*
- *Nonadiabatic Surface Chemistry*
- *Electronic Structure Theory and Methods*
- *Single Atom/Site Catalysis*
- *Electrocatalysis and Photocatalysis*

### 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*

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

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<sup>th</sup> 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**, 22<sup>nd</sup> 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

- 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\*** (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](https://doi.org/10.1038/s41467-018-07502-5).
- 32 Z. Li, S. Wang, and **H. Xin\*** (2018). "Toward artificial intelligence in catalysis". In: **Nat. Catal.** 1.9, pp. 641–642. doi: [10.1038/s41929-018-0150-1](https://doi.org/10.1038/s41929-018-0150-1).
- 31 S. Wang, N. Omidvar, E. Marx, and **H. Xin\*** (2018a). "Overcoming Site Heterogeneity In Search of Metal Nanocatalysts". In: **ACS Comb. Sci.** 20.10, pp. 567–572. doi: [10.1021/acscombsci.8b00070](https://doi.org/10.1021/acscombsci.8b00070).
- 30 Y. Lu, J. Wang, L. Yu, L. Kovarik, X. Zhang, A. Hoffman, A. Gallo, S. R. Bare, D. Sokaras, T. Kroll, V. Dagle, **H. Xin\***, and **A. M. Karim\*** (2018). "Identification of the Active Complex for CO Oxidation over Single-Atom Ir-on-MgAl<sub>2</sub>O<sub>4</sub> Catalysts". In: **Nat. Catal. (Accepted)**. doi: [10.1038/s41929-018-0192-4](https://doi.org/10.1038/s41929-018-0192-4).
- 29 Z. Li, N. Omidvar, W. S. Chin, E. Robb, A. Morris, L. Achenie, and **H. Xin\*** (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](https://doi.org/10.1021/acs.jpca.8b02842).
- 28 J. Wang, L. Yu, B. Hu, G. Chen, **H. Xin\***, and **X. Feng\*** (2018). "Efficient Electrohydrogenation of N<sub>2</sub> to NH<sub>3</sub> over Pd Catalyst at Low Overpotentials". In: **Nat. Commun.** 9.1, p. 1795. doi: [10.1038/s41467-018-04213-9](https://doi.org/10.1038/s41467-018-04213-9).
- 27 S. Wang, N. Omidvar, E. Marx, and **H. Xin\*** (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](https://doi.org/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](https://doi.org/10.1039/C7TA01812F).
- 25 S. Wang, J. Wang, and **H. Xin\*** (2017). "Insights into Electrochemical CO<sub>2</sub> 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](https://doi.org/10.1016/j.gee.2017.02.005).
- 24 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 CO<sub>2</sub> Reduction". In: **J. Am. Chem. Soc.** 139.5, pp. 1885–1893. doi: [10.1021/jacs.6b10435](https://doi.org/10.1021/jacs.6b10435).
- 23 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: [10.1016/j.cattod.2016.04.013](https://doi.org/10.1016/j.cattod.2016.04.013).
- 22 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: [10.1103/PhysRevLett.118.036101](https://doi.org/10.1103/PhysRevLett.118.036101).

- 21 **H. Xin\*** and S. Linic\* (2016). "Analyzing Relationships between Surface Perturbations and Local Chemical Reactivity of Metal Sites: Alkali Promotion of O<sub>2</sub> Dissociation on Ag(111)". In: **J. Chem. Phys.** 144.23, p. 234704. doi: [10.1063/1.4953906](https://doi.org/10.1063/1.4953906).
- 20 X. Ma, Z. Li, L. E. K. Achenie, and **H. Xin\*** (2015). "Machine-Learning-Augmented Chemisorption Model for CO<sub>2</sub> Electroreduction Catalyst Screening". In: **J. Phys. Chem. Lett.** Pp. 3528–3533. doi: [10.1021/acs.jpcllett.5b01660](https://doi.org/10.1021/acs.jpcllett.5b01660).
- 19 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](https://doi.org/10.1021/acscatal.5b00756).

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## Publications at Michigan, Stanford, and Tsinghua (China)

- 18 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: [10.1021/acs.jpcllett.7b01549](https://doi.org/10.1021/acs.jpcllett.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 (2016). "Chemical Bond Activation Observed with an X-ray Laser". In: **J. Phys. Chem. Lett.** 7.18, pp. 3647–3651. doi: [10.1021/acs.jpcllett.6b01543](https://doi.org/10.1021/acs.jpcllett.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\* (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).
- 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\* (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).
- 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](https://doi.org/10.1021/nl502571b).
- 13 **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).
- 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](https://doi.org/10.1021/ar3002393).
- 11 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).
- 10 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).

- 9 **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).
- 8 **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).
- 7 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).
- 6 **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).
- 5 **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).
- 4 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).
- 3 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.
- 2 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.
- 1 **H. Xin**, Q. Wu, M. Han\*, D. Wang, and Y. Jin (2005). "Alkylation of Benzene with 1-dodecene in Ionic Liquids [Rmim]<sup>+</sup>Al<sub>2</sub>Cl<sub>6</sub>X<sup>-</sup> (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).

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## Invited Lectures and Presentations

39. S. Wang, and **H. Xin\***, "Bayesian Chemisorption Theory of Catalysis", **ACS Spring Meeting**, Orlando, FL, 4/2019 (expected)
38. Zheng Li, S. Wang, and **H. Xin\***, "Machine Learning for Accelerating Discovery of Perovskite Electrocatalysts", **ACS Spring Meeting**, Orlando, FL, 4/2019 (expected)
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\***, "(Invited) Machine (& Human!) Learning in Catalyst Discovery", **XXVII International Materials Research Congress**, Cancun, Mexico, 8/2018
33. **H. Xin\***, "Overcoming Site Heterogeneity 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<sup>th</sup> 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<sub>x</sub> Interfaces for Electrochemical CO<sub>2</sub> 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 **16<sup>th</sup> 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<sub>2</sub> Reduction to C<sub>2</sub> Species", **AIChE Annual Meeting**, Salt Lake City, UT, 11/2015
7. **H. Xin\***, "CO<sub>2</sub> Electrocatalyst Design using a Hybrid Machine Learning and DFT Approach", **25<sup>th</sup> 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<sub>2</sub> 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

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## Research Group at Virginia Tech

### Current Members (7 PhD students, and 4 undergraduates)

- Zheng Li (PhD candidate, Jan. 2015 - May 2019 expected)
- Siwen Wang (PhD candidate, Aug. 2015 - May 2020 expected)
- Jiamin Wang (PhD student, Aug. 2015 - May. 2019 expected)
- 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 - )
- Junwei Luo (Undergraduate student, Feb. 2017 - )
- Emily Marx (Undergraduate student, May 2017 - )
- Bryan Ngo (Undergraduate student, Sep. 2017 - )
- Esther Robb (Undergraduate student, Nov. 2016 - )

### Previous Members (2 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
- Liang Yu (May 2017 - Mar. 2018), Dalian Institute of Chemical Physics

#### Awards for Group Students and Postdocs

- **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 252<sup>nd</sup> 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

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## Professional Services

### Conference Service

- 2017** Secretary of the Southeastern Catalysis Society.
- 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

- 2018** CHE Rep to 2018 AIChE Recruitment Fair.
- 2017** CHE Rep to the Engineering Faculty Organization (Alternative).

2017 Faculty Search Committee.

2015 Faculty Search Committee.

2014 Graduate Recruitment Committee.

2014 University Commencement Asst. Marshal.

### Teaching

- “Data Science for Chemical Engineers”, Virginia Tech, Spring 2019 expected
- “ChE Simulations”, Virginia Tech, Spring 2016, Spring 2017, Spring 2018
- “Computational Catalysis”, Virginia Tech, Fall 2016
- “Advanced Thermodynamics”, Virginia Tech, Fall 2014, Fall 2015, Fall 2018
- “Fundamental Catalysis”, Stanford University, Spring 2014
- “ChE Unit Operation”, University of Michigan, Ann Arbor, Spring 2010

### Review Service

- **Proposals:** NSF, ACS PRF, AFSOR, DoE
- **Journals:** 20+ journals including 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)