

Zhenghang Zhao, Ph.D.

Chemical and Biomolecular Engineering, University of Notre Dame
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EDUCATIONS

- **University of North Texas**, Denton, TX, USA Aug. 2012-May 2017
Ph.D. in Materials Science and Engineering
Dissertation Title: Design Principles on Carbon Nanomaterial Electrocatalysts for Energy Storage and Conversion
- **China University of Mining and Technology**, Beijing, China Sep. 2008-Jul. 2012
Bachelor of Engineering in Mechanical Engineering

RESEARCH EXPERIENCES

- **University of Notre Dame**, Notre Dame, IN, USA
Postdoctoral Research Associate with Prof. William F. Schneider Sep. 2018-Present
 - Performed large-scale DFT calculations and microkinetic modeling on the Cu exchange energies and citing preferences in CHA zeolites to analyze their activities as Selective Catalytic Reduction (SCR) catalysts;
 - Built a Monte Carlo model to predict the fraction of active Cu during transient and steady-state SCR. Discovered the SCR performance of zeolite is sensitive to the topology, ion siting, reaction condition, and framework heteroatoms;
 - Used molecular dynamics to calculate the interactions between the structure directing agents (SDA) and the framework heteroatoms, thus to predict the synthesis of zeolites.
- **Stanford University**, Stanford, CA, USA
Postdoctoral Research Fellow with Prof. Jens K. Nørskov Jun. 2017-Aug.2018
 - Performed large-scale high-throughput DFT screenings on unsupported and supported metal oxides to search for active ORR/OER electrocatalysts. Identified previously undiscovered Fe oxides as ORR electrocatalysts;
 - Used machine learning regression to predict the electrocatalytic activity of the materials with different descriptors;
 - Built a microkinetic model based on the calculated DFT results to predict the reaction rates of Co oxides as OER catalyst.
- **University of North Texas**, Denton, TX, USA
Research Assistant with Prof. Zhenhai Xia Aug. 2012-May 2017

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- For the first time, developed a novel descriptor, which was used as a design principle guiding the selection of proper carbon nanomaterials-based ORR/OER electrocatalyst. Discovered the synergistic effect between carbon substrates and the heteroatoms;
 - Conducted large-scale Density Functional Theory (DFT) calculations on carbon nanomaterials to investigate their electrocatalytic activities in oxygen reduction and evolution reactions (ORR/OER);
 - Collaborated with experimental groups by providing theoretical inputs to guide their experimental syntheses, and electrochemical tests on the carbon nanomaterials;
 - Collaborated with experimental groups by providing molecular dynamics simulation for the nanoindentation on Cu surface, identified dislocations generation and evolution mechanism.
- **China University of Mining and Technology**, Beijing, China
Undergraduate Research Assistant Sep. 2011-Jun. 2012
 - Performed experimental measurements on rocks under 3-dimensional pressure, identified stress-strain curve, and the mechanism of the deformation.

HIGHLIGHTS

- **19** publications: 1 book chapter and 18 peer-review journals including 1 *Nature Nanotechnology*, 5 *Advanced Materials*. (9 first authored/co-first authored)
- Total citation: 2170, H-index: 8. [Google Scholar](#)
- 4 invited talks from academia and national labs
- 15 conference and symposium proceedings

BOOK CHAPTER

Zhenghang Zhao, Lipeng Zhang, Chun-Yu Lin, Zhenhai Xia, Chapter 1: Design principles for heteroatom-doped carbon materials as metal-free catalysts. [Carbon-Based Metal-Free Catalysts: Design and Applications 1 \(2018\): 1-33](#).

JOURNAL PUBLICATIONS

1. **Zhenghang Zhao**, Philomena Schlexer Lamoureux, Ambarish Kulkarni, Michal Bajdich: Trends in Oxygen Electrocatalysis of 3d-Layered (Oxy)(Hydro)Oxides. *ChemCatChem*. 2019, 11 3423 [DOI: 10.1002/cctc.201900846](#)
2. **Zhenghang Zhao**, Jason D'Souza, Fuyi, Chen, Zhenhai Xia: Rational Design of Efficient Metallic Core-Shell Electrocatalysts for Oxygen Reduction and Evolution Reactions. *RSC Advances*. 2019, 9(1) 536. [DOI: 10.1039/c8ra09122f](#)

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3. **(Co-first)** J. Tyler Mefford, **Zhenghang Zhao**, Michal Bajdich, William C. Chueh: Rationalizing the Reactivity of Cobalt (Oxy)hydroxide Surfaces for Oxygen Evolution through Combined Thermodynamic and Kinetic Approaches. *Environmental & Energy Science*. (Under peer review)
4. Weiwei Zhao, Pallavi Bothra, Zhiyi Lu, Yanbin Li, Li-Pin Mei, Kai Liu, **Zhenghang Zhao**, et al: Improved Oxygen Reduction Reaction Activity of Nanostructured CoS₂ through Electrochemical Tuning. *ACS Applied Energy Materials*. ([Just Accepted](#))
5. Lipeng Zhang, Chun-Yu Lin, Detao Zhang, Lele Gong, Yonghao Zhu, **Zhenghang Zhao**, Quan Xu, Hejun Li, Zhenhai Xia: Guiding Principles for Designing Highly Efficient Metal-Free Carbon Catalysts. *Advanced Materials*. 2019, 31(13) 1805252. [DOI: 10.1002/adma.201805252](https://doi.org/10.1002/adma.201805252)
6. **Zhenghang Zhao**, Chun-Yu Lin, Jinlong Tang, Zhenhai Xia: Catalytic mechanism and design principles for heteroatom-doped graphene catalysts in dye-sensitized solar cells. *Nano Energy*. 2018, 49 193. [DOI: 10.1016/j.nanoen.2018.04.053](https://doi.org/10.1016/j.nanoen.2018.04.053)
7. **(Co-first)** Chun-Yu Lin, Detao Zhang, **Zhenghang Zhao**, Zhenhai Xia: Covalent Organic Framework Electrocatalysts for Clean Energy Conversion. *Advanced Materials*. 2018, 30(5) 1703646. [DOI: 10.1002/adma.201703646](https://doi.org/10.1002/adma.201703646)
8. Seoin Back, Martin H. Hansen, Jose A Garrido Torres, **Zhenghang Zhao**, Jens K. Nørskov, Samira Siahrostami, Michal Bajdich: Prediction of stable active oxyhydroxide nanoislands on transition metal supports. *ACS Applied Materials & Interfaces*. 2018, 11(2) 2006 [DOI: 10.1021/acsami.8b15428](https://doi.org/10.1021/acsami.8b15428)
9. **Zhenghang Zhao**, Zhenhai Xia: Rational Design of Novel Carbon Catalysts for Clean Energy Conversion and Storage. *Proceedings of the Nano-Micro Conference 2017*, 1(1) 01034. [DOI: 10.11605/cp.nmc2017.01034](https://doi.org/10.11605/cp.nmc2017.01034)
10. Chun-Yu Lin, Lipeng Zhang, **Zhenghang Zhao**, Zhenhai Xia: Design Principles for Covalent Organic Frameworks as Efficient Electrocatalysts in Clean Energy Conversion and Green Oxidizer Production. *Advanced Materials*. 2017, 29(17) 1606635. [DOI:10.1002/adma.201606635](https://doi.org/10.1002/adma.201606635)
11. **(Co-first)** Zhijuan Liu, **Zhenghang Zhao**, Yanyong Wang, Shuo Dou, Dafeng Yan, Dongdong Liu, Zhenhai Xia, Shuangyin Wang: In Situ Exfoliated, Edge-Rich, Oxygen-Functionalized Graphene from Carbon Fibers for Oxygen Electrocatalysis. *Advanced Materials*. 2017, 29(18) 1606207. [DOI:10.1002/adma.201606207](https://doi.org/10.1002/adma.201606207) (**Highly cited paper**)
12. Chun-Yu Lin, **Zhenghang Zhao**, Jianbing Niu, Zhenhai Xia: Synthesis, Properties and applications of 3D Carbon Nanotube-Graphene Junctions. *Journal of Physics D: Applied Physics*. 2016, 49(44) 443001. [DOI:49.44 \(2016\): 443001](https://doi.org/10.1088/0022-3719/49/44/443001)
13. **Zhenghang Zhao**, Zhenhai Xia: Design Principles for Dual-Element-Doped Carbon Nanomaterials as Efficient Bifunctional Catalysts for Oxygen Reduction and Evolution Reactions. *ACS Catalysis*. 2016, 6(3) 1553-1558. [DOI:10.1021/acscatal.5b02731](https://doi.org/10.1021/acscatal.5b02731)

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14. **Zhenghang Zhao**, Zhenhai Xia: Interactions between Dopants in Dual-Doped Graphene Nanoribbons as Metal-Free Bifunctional Catalysts for Fuel Cell and Metal-Air Batteries. *MRS Advances*. 2016, 1(6) 421. [DOI:10.1557/adv.2016.32](https://doi.org/10.1557/adv.2016.32)
15. **Zhenghang Zhao**, Lipeng Zhang, Zhenhai Xia: Electron Transfer and Catalytic Mechanism of Organic Molecule-Adsorbed Graphene Nanoribbons as Efficient Catalysts for Oxygen Reduction and Evolution Reactions. *The Journal of Physical Chemistry C*. 2016, 120(4) 2166. [DOI:10.1021/acs.jpcc.5b09611](https://doi.org/10.1021/acs.jpcc.5b09611)
16. **Zhenghang Zhao**, Mingtao Li, Lipeng Zhang, Liming Dai, Zhenhai Xia: Design Principles for Heteroatom-Doped Carbon Nanomaterials as Highly Efficient Catalysts for Fuel Cells and Metal-Air Batteries. *Advanced Materials*. 2015, 27(43) 6834. [DOI:10.1002/adma.201503211](https://doi.org/10.1002/adma.201503211)
(Highly cited paper)
17. Jintao Zhang, **Zhenghang Zhao**, Zhenhai Xia, Liming Dai: A metal-free bifunctional electrocatalyst for oxygen reduction and oxygen evolution reactions. *Nature Nanotechnology*, 2015, 10(5) 444. [DOI:10.1038/nnano.2015.48](https://doi.org/10.1038/nnano.2015.48) **(Most cited paper in 2015, Featured in phy.org)**
18. Reza A. Mirshams, **Zhenghang Zhao**, Zhiqiang Wang, Experimental Analysis and Computational Modeling of Pile-Up formation in Nanoindentation. *Mex. J. Mat. Sci. Eng.* 1 (2014) 1-11.

INVITED TALKS

1. DFT Investigations of Novel Materials in Electrochemical Catalysis, Invited talk, National Renewable Energy Laboratory, Golden, CO, Jun. 2018
2. Theoretical Investigations of Chemical Reactions in Energy Storage and Conversion, Invited talk, Carnegie Mellon University, Pittsburgh, PA, May. 2018
3. Understanding the Heterogeneous Catalysis in Energy Storage and Conversion, Invited talk, Lawrence Livermore National Laboratory, Livermore, CA, USA. May. 2018
4. Catalytic Mechanisms of Doped Graphene as Efficient Bifunctional Catalysts for Fuel Cells and Metal-air Batteries, Invited Talk, Southeastern Louisiana University, Hammond, LA, USA, Apr. 2016

CONFERENCES & SYMPOSIUM

1. Trends in Oxygen Electrocatalysis of 3d-Layered (Oxy)(Hydro)Oxides. 2019 AIChE Annual Meeting, Orlando, FL, Nov. 2019
2. First-principle Investigation of Cu Ion Exchange and Siting Preference in Ferrierite. 2019 AIChE Annual Meeting, Orlando, FL, Nov. 2019
3. First-principle Investigation of Cu Ion Exchange and Siting Preference in Ferrierite, NAM26 2019 North American Catalysis Society Meeting, Chicago, IL, Jun. 2019

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4. First-Principles Investigation of Cu Ion Exchange and Siting Preference in Selected Zeolite Topologies, 2019 Chicago Catalysis Club Symposium, Chicago, IL, Apr. 2019
5. High-Throughput Catalysts Screening of Layered Double Hydroxides for Oxygen Evolution and Reduction Reactions, 2018 AIChE Annual Meeting, Pittsburgh, PA, Oct. 2018
6. Trends in Electrochemical Oxygen Reduction and Evolution Activities of Layered Double Hydroxides, CBE Symposium, University of Notre Dame, IN, Sep. 2018
7. Trends in Electrochemical Oxygen Reduction and Evolution Activities of Layered Double Hydroxides, SUNCAT Industry Affiliates meeting, Stanford, CA, Jun. 2018
8. Co-doped Carbon Nitride Single-atom Catalyst for Oxygen Reduction Reaction, TRI conference, San Mateo, CA, May. 2018
9. High-throughput Catalysts Screening of Layered Double Hydroxides for Oxygen Evolution and Reduction Reactions, The MRS Spring Meeting, Phoenix, AZ, Apr. 2018
10. High-throughput Catalysts Screening of Layered Double Hydroxides for Oxygen Evolution and Reduction Reactions, Oral Presentation, APS March Meeting 2018, Los Angeles, CA, USA, Mar. 2018
11. Catalytic Mechanism of the Oxygen Reduction and Evolution Reactions on Co-doped g-C₃N₄, SUNCAT Summer Institute, Menlo Park, CA, Aug. 2017
12. Catalytic Mechanism and Design Principles for Heteroatom-Doped Graphene Catalysts in Dye-Sensitized Solar Cells, AMMPI Industry Workshop, Denton, TX, May. 2017
13. Catalytic Mechanism and Design Principles for Heteroatom-Doped Graphene Catalysts in Dye-Sensitized Solar Cells, The MRS 2017 Spring conference, Phoenix, AZ, Apr. 2017
14. Catalytic Mechanisms of Doped Graphene as Efficient Catalysts for Fuel Cells and Metal-air Batteries, Technical Presentation, IMECE 2015, ASME conference, Houston, TX, USA, Nov. 2015
15. Carbon-based Bifunctional Catalysts for Fuel Cells and Metal-air Batteries, Graduate Seminar Showcase, University of North Texas, Denton, TX, USA, Apr. 2015
16. Nanoindentation on FCC Nickel for Different Crystalline Orientation Using Molecular Dynamics Method, The Second International Conference on Metallic Materials and Processing, Las Vegas, NV, USA, Oct. 2014
17. Nanoindentation on FCC Nickel for Different Crystalline Orientation Using Molecular Dynamics Method, CASCaM, University of North Texas, Denton, TX, USA, Sep. 2013

AWARDS

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Raupe Travel Grant, University of North Texas, 2017

Graduate Fellowship, Advanced Materials Manufacturing Processes Institute, 2015

MEMBERSHIP, SERVICES & LANGUAGES

- **Membership:**

American Institute of Chemical Engineers (AIChE)

Materials Research Society (MRS)

- **Services:**

Editorial board: *Polymer, Frontier in Materials*

Journal reviewer: *Journal of American Chemical Society, Advanced Energy Materials, ACS Catalysis, ACS Applied Materials and Interfaces, Journal of Physical Chemistry C, Materials, Polymers, Energies, Catalysts, Sustainability, Computational Materials Science, International Journal of Quantum Chemistry, ACS Omega, Journal of Bionic Engineering, Chemical Physics Letters, Nanomaterials, etc.*

Conference organizer: The Second International Conference on Metallic Materials and Processing, Las Vegas, NV, USA, Oct. 2014

Judge: Undergraduate poster session, 2019 AIChE Annual Meeting, Orlando, FL, Nov. 2019

- **Languages:**

English (full professional working fluency) and Mandarin Chinese (native)

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