

# ZISHENG ZHANG · 張 孜 晟

Email: zisheng@chem.ucla.edu ♦ Website: zishengz.github.io ♦ Tel: +1 (424) 535-9227

3607 Greystone Drive, Apt #2020, Austin, TX, 78731, United States

## EDUCATION

<b>University of California, Los Angeles (UCLA)</b>	Apr 2021 - Jun 2024 (ABD)
Ph. D. Candidate in Chemistry, Theoretical & Computational	Advisor: Anastassia N. Alexandrova
<b>University of California, Los Angeles (UCLA)</b>	Sep 2019 - Mar 2021
M. Sc. in Chemistry, Theoretical & Computational	Advisor: Anastassia N. Alexandrova
<b>Southern University of Science and Technology (SUSTech)</b>	Sep 2015 - Jun 2019
B. Sc. in Chemistry <i>summa cum laude</i> (Rank 1/75 in the program)	Advisor: Jun Li

## SCHOLARSHIPS & AWARDS

Dissertation Year Fellowship, UCLA	Oct 2023
Jim and Barbara Tsay Excellence in Research Award, UCLA	May 2023
CATL-ChemCatBio Graduate Student Travel Award, ACS CATL division	Mar 2023
CCG Excellence Award for Graduate Students, ACS COMP division	Mar 2023
Best Poster Award in graduate student division, Gordon Research Conference on Catalysis	Jul 2022
Jim and Barbara Tsay Excellence in 2 <sup>nd</sup> Year Research and Academics Award, UCLA	May 2022
Edwin W. Pauley Fellowship, UCLA	Feb 2020
Outstanding B.Sc. Thesis Award, SUSTech	Jun 2019
Graduate Dean's Scholar Award, UCLA	Apr 2019
Best Presentations Award in CSST CHEM & MSE division, UCLA	Sep 2018
Cross-disciplinary Scholar in Science and Technology (CSST) Fellowship, UCLA	Jul 2018
Undergraduate Scholarship, SUSTech	2016, 2017, 2018

## WORK & RESEARCH EXPERIENCE

<b>Department of Chemistry and Biochemistry, UCLA</b>	Sep 2019 - Present
Advisor: Prof. Anastassia N. Alexandrova & Prof. Philippe Sautet	Graduate Student Researcher
<ul style="list-style-type: none"><li>• Develop a global optimizer for minima search and configurational sampling of supported metal clusters, micro-solvated interface, off-stoichiometric surface reconstruction, and adsorbate coverage/configurations.</li><li>• Grand canonical ensemble representation of fluxional clusters and surfaces in catalytic conditions.</li><li>• Inverse molecular design of electrochemical CO<sub>2</sub> capturing agents (organic and organometallic) by electronic structure calculation, multi-objective global optimization, and machine learning.</li><li>• Realistic modeling of electrochemical interface to understand the role of pH, cations, potential, and surface modification in alkaline hydrogen electrocatalysis by explicit solvation and constant potential MD.</li></ul>	
<b>Center for Nanoscale Materials, Argonne National Laboratory</b>	Jun 2022 - Sep 2022
Supervisor: Dr. Maria K. Chan	Research Aide Technical - Ph.D. level
<ul style="list-style-type: none"><li>• Develop an experiment-informed multi-objective global optimizer for crystal structure prediction.</li></ul>	
<b>Department of Chemistry and Biochemistry, UCLA</b>	Jun 2018 - Dec 2018
Supervisor: Prof. Anastassia N. Alexandrova	CSST Summer Fellow
<ul style="list-style-type: none"><li>• Mechanistic study of thermal- and electrocatalysis on borides, focusing on metastable surface states.</li></ul>	

- Dynamics and free energetics of single atom electrocatalysis from *ab initio* MD with explicit electrolyte.
- Molecular design of transition metal phthalocyanine-based catalysts for electrocatalytic CO<sub>2</sub>RR and 2/4e<sup>-</sup> ORR by mechanistic study, high-throughput computation, global optimization, and machine learning.

## PUBLICATIONS

**Total citations: 2096; h-index: 17** (Google Scholar, Mar 2024); <sup>1</sup> = co-first authorship; \* = corresponding.

Selected<sup>Δ</sup>: #29 *Nat.Mater.*, #8 & #25 *ACIE*, #21 & #31 & #36 *JACS*, #20 *Nat.Catal.*, #19 *Chem.Soc.Rev.*, #17 *PNAS*, #15 *Nat.Comm.*, #7 & #34 *Acc.Chem.Res.*

36. Δ Shah, A. H.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Wan, C.; Wang, S.; Zhang, A.; Wang, L.; Alexandrova, A. N.\*; Huang, Y.\*; Duan, X.\* The platinum-surface water orientation dictates hydrogen evolution reaction kinetics in alkaline media. *J. Am. Chem. Soc.*, **2024**, Accepted.
35. Yan, H.-M.; **Zhang, Z.**; Wang, Y.-G.\* Coverage-Induced Cation Dehydration and Migration for Enhanced CO–CO Coupling on Cu Electrocatalysts. *ACS Catal.*, **2024**, *14*, 3596-3605.
34. Δ **Zhang, Z.**; Li, J.; Wang, Y.-G.\* Modeling Interfacial Dynamics on Single Atom Electrocatalysts: Explicit Solvation and Potential Dependence. *Acc. Chem. Res.*, **2024**, *57*, 198-207.
33. Cendejas, M.; Mellone, O. A. P.; Unni, K.; **Zhang, Z.**; Jacob, J.; Ibrahim, F.; Dong, S.; Vinson, J.; Alexandrova, A. N.; Sokaras, D.\*; Bare, S. R.\*; Hermans, I.\* Tracking Active Phase Behavior on Boron Nitride during the Oxidative Dehydrogenation of Propane Using Operando X-Ray Raman Spectroscopy. *J. Am. Chem. Soc.*, **2023**, *145*, 25686-25694.
32. Yu, Y.<sup>1</sup>; Koh, H.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Yang, Z.; Alexandrova, A. N.; Stach, E. A.\*; Xie, J.\* Kinetic Pathways of Fast Lithium Transport in Solid Electrolyte Interphases with Discrete Inorganic Components. *Energy Environ. Sci.*, **2023**, *16*, 5904-5915.
31. Δ **Zhang, Z.**; Hermans, I.; Alexandrova, A. N.\* Off-stoichiometric Restructuring and Sliding Dynamics of Hexagonal Boron Nitride Edges in Conditions of Oxidative Dehydrogenation of Propane. *J. Am. Chem. Soc.*, **2023**, *145*, 17265-17273.
30. Zheng, H.; Li, H.; **Zhang, Z.**; Wang, X.; Jiang, Z.; Tang, Y.; Zhang, J.; Emley, B.; Zhang, Y.; Zhou, H.; Yao, Y.\*; Liang, Y.\*. Dispersed Nickel Phthalocyanine Molecules on Carbon Nanotubes as Cathode Catalysts for Li-CO<sub>2</sub> Batteries. *small*, **2023**, accepted, DOI: 10.1002/smll.202302768.
29. Δ Wan, C.; **Zhang, Z.**; Dong, J.; Xu, M.; Pu, H.; Baumann, D.; Lin, Z.; Wang, S.; Huang, J.; Shah, A. H.; Pan, X.; Hu, T.; Alexandrova, A. N.\*; Huang, Y.\*; Duan, X.\* Creating a local acidic environment on platinum surface for high-performance hydrogen evolution reaction in alkaline electrolyte. *Nat. Mater.*, **2023**, *22*, 1022-1029.
28. Zito, A.; Clarke, L.; Barlow, J.; Daniel, B.; **Zhang, Z.**; Ripley, K.; Li, C.; Kummeth, A.; Leonard, M.; Alexandrova, A. N.\*; Brushett, F.\*; Yang, J. Y.\* Electrochemical Carbon Dioxide Capture and Concentration. *Chem. Rev.*, **2023**, *123*, 8069-8098.
27. Cao, H.; Wang, Q.; **Zhang, Z.**; Yan, H.-M.; Zhao, H.; Yang, H. B.; Liu, B.\*; Li, J.; Wang, Y.-G.\* Engineering Single-Atom Electrocatalysts for Enhancing Kinetics of Acidic Volmer Reaction. *J. Am. Chem. Soc.*, **2023**, *145*, 13038-13047.

26. Cheng, D.; Wei, Z.; **Zhang, Z.**; Broekmann, P.; Sautet, P.\*; Alexandrova, A. N.\* Restructuring and Activation of Cu(111) under Electrocatalytic Reduction Conditions. *Angew. Chem., Int. Ed.*, **2023**, 62, e202218575.
25. Δ **Zhang, Z.**<sup>1</sup>; Masubuchi, T.<sup>1</sup>; Sautet, P.; Anderson, S. L.\*; Alexandrova, A. N.\* Hydrogen Evolution on Electrode-Supported Ptn Clusters: Ensemble of Hydride States Governs the Size Dependent Reactivity. *Angew. Chem., Int. Ed.*, **2023**, 62, e202218210.
24. Poths, P.; Li, G.; Masubuchi, T.; Morgan, H. T.; **Zhang, Z.**; Alexandrova, A. N.\*; Anderson, S. L.\* Got Coke? Self-Limiting Poisoning Makes an Ultra Stable and Selective Sub-nano Cluster Catalyst. *ACS Catal.*, **2023**, 13, 1533-1544.
23. Jiang, Z.; **Zhang, Z.**; Li, H.; Tang, Y.; Yuan, Y.; Zao, J.; Zheng, H.; Liang, Y.\* Molecular Catalyst with Near 100% Selectivity for CO<sub>2</sub> Reduction in Acidic Electrolytes. *Adv. Energy Mater.*, **2022**, 13, 2203603.
22. Munarriz, J.; **Zhang, Z.**; Sautet, P.\*; Alexandrova, A. N.\* Graphite-supported Ptn Cluster Electrocatalysts: Major Change of Active Sites as a Function of the Applied Potential. *ACS Catal.*, **2022**, 12, 14517-14526.
21. Δ **Zhang, Z.**; Wei, Z.; Sautet, P.\*; Alexandrova, A. N.\* Hydrogen-induced Restructuring of a Cu(100) Electrode in Electroreduction Conditions. *J. Am. Chem. Soc.*, **2022**, 144, 19284-19293
20. Δ Shah, A. H.; **Zhang, Z.**; Huang, Z.; Wang, S.; Zhong, G.; Wan, C.; Alexandrova, A. N.; Huang, Y.; Duan, X.\* Unriddling the role of alkali metal cations and surface hydroxide in alkaline hydrogen evolution reaction. *Nat. Catal.*, **2022**, 5, 923-933.  
- Featured in *Nat. Catal. News & Views*
19. Δ Barlow, J. M.<sup>1</sup>; Clarke, L.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Daniel, B.; Leonard, M.; Zito, A.; Brushett, F.\*; Alexandrova, A. N.\*; Yang, J. Y.\* Molecular Design of Redox Carriers for Electrochemical CO<sub>2</sub> Capture and Concentration. *Chem. Soc. Rev.*, **2022**, 51, 8415-8433.
18. Zhao, H.; Cao, H.; **Zhang, Z.**; Wang, Y.-G.\* Modelling the Potential Dependent Kinetics of CO<sub>2</sub> Electroreduction on Single Nickel Atom Catalyst with Explicit Solvation. *ACS Catal.*, **2022**, 12, 11380-11390.
17. Δ **Zhang, Z.**; Kummeth, A. L.; Yang, J. Y.\*; Alexandrova, A. N.\* Inverse Molecular Design of Alkoxides and Phenoxides for Aqueous Direct Air Capture of CO<sub>2</sub>. *Proc. Nat. Acad. Sci.*, **2022**, 119, e2123496119
16. Cao, H.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Chen, J. W.; Wang, Y.-G.\* Potential Dependent Free Energy Relationship in Interpreting the Electrochemical Performance of CO<sub>2</sub> Reduction on Single Atom Catalyst. *ACS Catal.*, **2022**, 12, 6606-6617.
15. Chen, J.W.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Yan, H.<sup>1</sup>; Xia, G.-J.; Cao, H.; Wang, Y.-G.\* Pseudo-adsorption and Long-range Redox Coupling during Oxygen Reduction Reaction on Single Atom Electrocatalyst. *Nat. Commun.*, **2022**, 13, 1-13.
14. **Zhang, Z.**; Zandkarimi, B.; Munarriz, J.; Dickerson, C.; Alexandrova, A. N.\* Fluxionality of Subnano Clusters Reshapes the Activity Volcano of Electrocatalysis. *ChemCatChem*, **2022**, 14, e202200345.  
- Special issue: Catalysts and Reactors under Dynamic Conditions for Energy Storage and Conversion
13. Lavroff, R. H.; Morgan H. W.T.; **Zhang, Z.**; Poths, P.; Alexandrova, A. N.\* Ensemble Representation of Catalytic Interfaces: Soloists, Orchestras, and Everything In-between. *Chem. Sci.*, **2022**, 13, 8003-8016.

12. Wang, Y.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Zhang, X.; Yuan, Y.; Zhan, J.; Zheng, H.; Wang, Y.-G.; Zhou, H.; Liang, Y. Theory-driven design of electrocatalysts for the two-electron oxygen reduction reaction based on dispersed metal phthalocyanines. *CCS Chem.*, **2022**, *4*, 585-593.
11. **Zhang, Z.**; Wang, Y.-G.\* Molecular Design of Nickel Phthalocyanine@Nanocarbon Hybrid Single-atom Catalyst for Active and Stable Electroreduction of CO<sub>2</sub>. *J. Phys. Chem. C*, **2021**, *125*, 13836-13849.  
- Special issue: Energy and Catalysis in China
10. **Zhang, Z.**; Cui, Z.-H.; Jimenez-Izal, E.; Sautet, P.\*; Alexandrova, A. N.\* Hydrogen Evolution on Re-structured B-rich WB: Metastable Surface States and Isolated Active Sites. *ACS Catal.*, **2020**, *10*, 13867-13877.
9. Zhang, X.<sup>1</sup>; Wang, Y.<sup>1</sup>; Gu M.<sup>1</sup>; Wang, M.<sup>1</sup>; **Zhang, Z.**; Pan, W.; Jiang, Z.; Zheng, H.; Lucero, M.; Wang, H.; Sterbinsky, G.; Ma, Q.; Wang, Y.-G.\*; Feng, Z.\*; Li, J.; Dai, H.; Liang, Y.\* Molecular Engineering of Dispersed Nickel Phthalocyanines on Carbon Nanotubes for Selective CO<sub>2</sub> Reduction. *Nat. Energy*, **2020**, *5*, 684-692.
8. Δ Venegas, J.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Agbi, T.; McDermott, W.; Alexandrova, A. N.\*; Hermans, I.\* Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane. *Angew. Chem., Int. Ed.*, **2020**, *59*, 16527-16535.  
- Designated as a "Very Important Paper (VIP)" article by evaluators
7. Δ **Zhang, Z.**; Zandkarimi, B.; Alexandrova, A. N.\* Ensembles of metastable states govern heterogeneous catalysis on dynamic interfaces. *Acc. Chem. Res.*, **2020**, *53*, 447-458.
6. Wang, Y.; Wang, M.; **Zhang, Z.**; Wang, Q.; Jiang, Z.; Lucero, M.; Zhang, X.; ; Li, X.; Gu, M.\*; Feng, Z.\*; Liang, Y.\* Iron Phthalocyanine Precursors to Construct Efficient Single Iron Site Electrocatalysts for Oxygen Reduction Reaction. *ACS Catal.*, **2019**, *9*, 6252-6261.
5. Zhong, R.; **Zhang, Z.**; Luo, S.; Zhang, Z. C.; Huang, L.\*; Gu, M.\* Comparison of TiO<sub>2</sub> and g-C<sub>3</sub>N<sub>4</sub> 2D/2D Nanocomposites from Three Synthesis Protocols for Visible-light Induced Hydrogen Evolution. *Catal. Sci. Technol*, **2019**, *9*, 75-85.  
- Front cover highlight
4. **Zhang, Z.**; Jimenez-Izal, E.; Hermans, I.; Alexandrova, A. N.\* Dynamic Phase Diagram of Catalytic Surface of Hexagonal Boron Nitride in Conditions of Oxidative Dehydrogenation of Propane. *J. Phys. Chem. Lett.* **2018**, *10*, 20-25.
3. Zhong, R.<sup>1</sup>; **Zhang, Z.**<sup>1</sup>; Yi, H.; Zeng, L.; Tang, C.; Huang, L.\*; Gu, M.\* Covalently Bonded 2D/2D O-g-C<sub>3</sub>N<sub>4</sub>/TiO<sub>2</sub> Heterojunction for Enhanced Visible-Light Photocatalytic Hydrogen Evolution. *Appl. Catal. B*, **2018**, *237*, 1130-1138.
2. **Zhang, Z.**; Yang, T.; Qin, P.; Dang, L.\* Nickel Bis(dithiolene) Complexes for Electrocatalytic Hydrogen Evolution: A Computational Study. *J. Organomet. Chem.*, **2018**, *864*, 143-147.  
- Special issue: Modern Computational Organometallic Chemistry
1. Zhang, X.; Wu, Z.; Zhang, X.; Li, L.; Li, Y.; Xu, H.; Li, X.; Yu, X.; **Zhang, Z.**; Liang, Y.\* and Wang, H.\* Highly Selective and Active CO<sub>2</sub> Reduction Electrocatalysts Based on Cobalt Phthalocyanine/carbon Nanotube Hybrid Structures. *Nat. Commun.* **2017**, *8*, 14675.
- ?. Qie, B.; Wang, Z.; Jiang, J.; **Zhang, Z.**; Jacobse, P. H.; Lu, J.; Li, X.; Liu, F.; Alexandrova, A. N.; Louie, S.

G.\*; Crommie, M. F.\*; Fischer, F. R.\* Low Dimensional N-Heterocyclic Carbene-Metal Lattices. Under Review.

## PRESENTATIONS

---

12. "Grand Canonical Ensemble Representation of Dynamic Catalysts: From Thermal to Electro, From Clusters to Surfaces" Invited Talk, *Liu Group Seminar*; Austin, TX, United States; Feb, 2024.
11. "Grand Canonical Ensemble Representation of Dynamic Catalysts: From Thermal to Electro-catalysis, From Clusters to Surfaces" Dissertation Talk, *Exit Seminar*; Los Angeles, CA, United States; Nov 2023.
10. "Unriddling the cationic and pH effect in alkaline hydrogen evolution reaction on Pt" Oral Presentation, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.
9. "Inverse molecular design of alkoxides and phenoxides for aqueous direct air capture of CO<sub>2</sub>" Oral Presentation, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.
8. "Modeling fluxionality and off-stoichiometric restructuring at electrochemical interfaces." Poster Presentations, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.  
- ACS COMP - CCG Excellence in Research Award Symposium
7. "Modeling Fluxionality and Off-Stoichiometric Restructuring at Electrochemical Interfaces." Virtual Poster Presentation, *#RSCPoster Twitter Conference*; link; Mar 2023.
6. "Modeling Catalysis the Hard Way: Grand Canonical Ensemble Representation of Catalytic Interfaces." Invited Talk, *Henkelman Group Seminar*; Austin, TX, United states; Oct 2022.
5. "Modeling Fluxionality and Off-Stoichiometric Restructuring at Electrochemical Interfaces." Poster Presentations, *Gordon Research Seminar & Conference on Catalysis*; New London, NH, United States; Jun 2022.  
- Best Graduate Student Poster Award at Gordon Research Conference
4. "Inverse Molecular Design of Alkoxide and Phenoxide for Aqueous CO<sub>2</sub> Capture." Oral Presentation, *Sloan Annual Meeting: CO<sub>2</sub> capture*; Irvine, CA, United States; Mar 2022.
3. "Resolving Active Sites of Hexagonal Boron Nitride for Oxidative Dehydrogenation of Propane: A Computational Study." Poster and Oral Presentation, *Cross-disciplinary Scholars in Science and Technology Peer Seminar*; Los Angeles, CA, United States; Sep 2018.
2. "Bimetallic Copper/Palladium Nanoparticles Anchored on Carbon Nanotube for Selective Electrorreduction of Carbon Dioxide." Poster Presentation, *Nature Conference: Material Electrochemistry*; Shenzhen, Guangdong, China; Jan 2018.
1. "Designing High-performance Nickel Bis(substituted-dithiolene) Electrocatalysts for HER - A Computational Study." Oral Presentation, *ACS Symposium: Innovation in Energy Conversion*; Dalian, Liaoning, China; Sep 2017.

## TEACHING

---

Teaching Assistant of Chemistry 126/226: Computational Methods for Chemists, UCLA	Spring 2022
Exploring Your Universe Educational Event - Computational Chemistry Booth, UCLA	Nov 2021
Teaching Assistant of Chemistry 17: Chemical Principles, UCLA	Winter 2020
Teaching Assistant of Chemistry 30AL: General Chemistry Lab II, UCLA	Fall 2019

## RESEARCH MENTORING

---

<b>Anubhav Goswami</b> , Ph.D. Student (Chemistry), UCLA	2023 - Present
<b>Dylan Karkainen</b> , Undergraduate (Chemistry), UCLA	2023 - Present
<b>Jack Cokas</b> , Undergraduate (Chemistry), UCLA	2023 - Present
<b>Shawn Chiu</b> , Ph.D. Student (Chemistry), UCLA	2022 - Present
<b>Samuel Greenbank</b> , Undergraduate (visiting), UCLA	2022 - 2023
<b>Robert Lavroff</b> , Ph.D. Student (Chemistry), UCLA	2021 - Present
<b>Winston Gee</b> , Ph.D. Student (Chemistry), UCLA	2021 - Present
<b>Edison Cummings</b> , Undergraduate (Chemistry), UCLA	2022 - Present
<b>Jennifer Tjia</b> , Undergraduate (Chemistry), UCLA	2022 - 2023
<b>Tom Z. Hong</b> , Undergraduate (Mathematics), UCLA	2022 - 2023

## PROFESSIONAL SERVICES

---

### Affiliations:

Member of American Chemical Society (COMP & CATL)	2018 - Present
Vice Chair of ACS Student Chapter, SUSTech	2018 - 2019
Academic Division Chair of MRS Student Chapter, SUSTech	2018 - 2019

### Reviewing Services:

(41 completed journal reviews, Web of Science Statistics, updated Mar 2024)	
Reviewer of Journal of the American Chemical Society (ACS)	2024 - Present
Reviewer of The New Journal of Chemistry (RSC)	2024 - Present
Reviewer of GenBio@NeurIPS	2023
Reviewer of The Journal of Physical Chemistry C (ACS)	2020 - Present
Reviewer of Computational and Theoretical Chemistry (Elsevier)	2021
Reviewer of ACS In Focus series (ACS)	2021