

# ZISHENG ZHANG · 張 孜 晟

Email: zisheng@chem.ucla.edu ♦ Website: zishengz.github.io ♦ Tel: +1 (424) 535-9227  
Young Hall 3051, 607 Charles E. Young Drive East, Los Angeles, CA, 90025, United States

## EDUCATION

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

## SCHOLARSHIPS & AWARDS

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> Advisor: Prof. Anastassia N. Alexandrova & Prof. Philippe Sautet	Sep 2019 - Present 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 on Pt by explicit solvation and constant potential treatments.</li></ul>	
<b>Center for Nanoscale Materials, Argonne National Laboratory</b> Supervisor: Dr. Maria K. Chan	Jun 2022 - Sep 2022 Research Aide Technical - Ph.D. level
<ul style="list-style-type: none"><li>Develop an experiment-informed multi-objective global optimizer for structure search of bulk and 2D materials.</li></ul>	
<b>Department of Chemistry and Biochemistry, UCLA</b> Supervisor: Prof. Anastassia N. Alexandrova	Jun 2018 - Dec 2018 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>	
<b>Department of Chemistry, SUSTech</b> Advisor: Prof. Jun Li & Prof. Yang-Gang Wang	Sep 2018 - Jun 2019 Undergraduate Researcher
<ul style="list-style-type: none"><li>Dynamics and free energetics of single atom electrocatalysis from <i>ab initio</i> MD simulation with explicit electrolyte.</li><li>Molecular design of transition metal phthalocyanine-based electrocatalysts for electrocatalytic CO<sub>2</sub>RR and 2/4e<sup>-</sup> ORR by mechanistic study, high-throughput computation, global optimization, and machine learning.</li></ul>	

## PUBLICATIONS

- Total citations: 1414; h-index: 11** (Google Scholar Statistics, Mar 2023); <sup>1</sup> = co-first authorship; \* = corresponding.  
Selected: #26 *ACIE*, #21 *JACS*, #20 *Nat. Catal.*, #19 *Chem. Soc. Rev.*, #17 *PNAS*, #15 *Nat. Commun.*, #8 *ACIE*, #7 *Acc. Chem. Res.*
26. **Zhang, Z.**<sup>1</sup>; Masubuchi, T.<sup>1</sup>; Sautet, P.; Anderson, S. L.\*; Alexandrova, A. N.\* *Angew. Chem., Int. Ed.*, **2023**, accepted, preprint on ChemRxiv.
  25. Cheng, D.; Wei, Z.; **Zhang, Z.**; Broekmann, P.; Sautet, P.\*; Alexandrova, A. N.\* *Angew. Chem., Int. Ed.*, **2023**, accepted.
  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. **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. Shah, A.; **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. 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. **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 Restructured 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. 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. **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.*, *864*, **2018**, 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.
- ?. 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.\* Under Review, preprint on ChemRxiv.

## PRESENTATIONS

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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 Electroreduction 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

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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

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<b>Shawn Chiu</b> , Ph.D. Student (Chemistry), UCLA	2022 - Present
<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 - Present

## PROFESSIONAL SERVICES

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<b>Affiliations:</b>	
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
<b>Reviewing Services:</b>	
(30 completed journal reviews, Web of Science Statistics, updated Mar 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

## REFERENCES

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1. **Dr. Jun Li** junli@mail.tsinghua.edu.cn  
Professor, Department of Chemistry  
Tsinghua University; Beijing, China
  2. **Dr. Anastassia N. Alexandrova** ana@chem.ucla.edu  
Professor, Department of Chemistry and Biochemistry  
University of California, Los Angeles; Los Angeles, CA, United States
  3. **Dr. Philippe Sautet** sautet@ucla.edu  
Professor, Department of Chemistry and Biochemistry  
University of California, Los Angeles; Los Angeles, CA, United States
  4. **Dr. Maria K. Chan** mchan@anl.gov  
Scientist, Center for Nanoscale Materials  
Argonne National Laboratory; Lemont, IL, United States