

ZISHENG ZHANG · 張 孜晟

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Young Hall 3051, 607 Charles E. Young Drive East, Los Angeles, CA, 90025, United States

EDUCATION

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| University of California, Los Angeles | Apr 2021 - Present |
| Ph.D. Candidate, Theoretical/Computational Chemistry | GPA 3.90/4.00 |
| University of California, Los Angeles | Sep 2019 - Mar 2021 |
| Master of Science, Theoretical/Computational Chemistry | GPA 3.87/4.00 |
| Southern University of Science and Technology (SUSTech) | Sep 2015 - Jun 2019 |
| Bachelor of Science, Chemistry | GPA 3.87/4.00 (Ranking: 1/75) |
| University of California, Los Angeles | Jul 2018 - Sep 2018 |
| Cross-disciplinary Scholar in Science and Technology (CSST) | GPA 4.00/4.00 (Ranking: 1/101) |

RESEARCH EXPERIENCE

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| Department of Chemistry and Biochemistry, UCLA | Sep 2019 - Present |
| Advisor: Prof. Anastassia Alexandrova and Prof. Philippe Sautet | Graduate Student Researcher |
| <ul style="list-style-type: none">· Mechanistic study of heterogeneous catalysis and electrocatalysis on borides based on metastable surface states.· Modeling electrocatalysis on Pt₁₋₇@FTO with global optimization and grand canonical DFT calculation.· Molecular engineering of metal-alkoxide carrier system for electrochemical capturing and conversion of CO₂ with electronic structure calculation (semi-empirical QM and DFT), genetic algorithms and machine learning.· Grand Canonical Genetic Algorithm for minima search of restructured and adsorbate-covered catalytic interfaces. | |
| Department of Chemistry and Biochemistry, UCLA | Jun 2018 - Dec 2018 |
| Advisor: Prof. Anastassia Alexandrova | CSST Summer Fellow |
| <ul style="list-style-type: none">· Modeled the dynamic boride surface in catalytic condition with Particle Swarm Optimization, DFT calculation, and BOMD. Establishing a grand canonical ensemble to study ensemble-averaged surface free energy and Bader charge, revealing metastable active sites with unusual bonding environments. | |
| Department of Chemistry, SUSTech | Sep 2018 - Jun 2019 |
| Advisor: Prof. Jun Li and Prof. Yang-Gang Wang | Undergraduate Researcher |
| <ul style="list-style-type: none">· Applied high-throughput DFT and semi-empirical calculations to study the substituent group effects on the activity and stability of nickel phthalocyanine (NiPc) derivatives for selective electroreduction of CO₂ to CO. | |
| Department of Material Science and Engineering (MSE), SUSTech | Jun 2016 - Jun 2019 |
| Advisor: Prof. Yongye Liang | Undergraduate Researcher |
| <ul style="list-style-type: none">· Applied DFT calculations to investigate the molecular engineering of FePc derivatives for oxygen reduction reaction. Constructed FePc/CNT hybrids to enhance electrocatalytic activity and stability.· Fabricated single-atom catalysts through pyrolysis of ZIF-8 encapsulated metal phthalocyanine for ORR.· Designed and synthesized bimetallic Cu/Pd NPs supported on oxidized CNT via an adopted co-strong electrostatic adsorption method, achieving selective CO₂RR to formic acid in a wide potential range. | |

- Synthesized and tested CoPc/CNT hybrids for selective electrocatalytic reduction of CO₂.

Department of Chemistry & Department of MSE, SUSTech

May 2017 - Oct 2018

Advisor: Prof. Limin Huang and Prof. Meng Gu

Undergraduate Researcher

- Designed and synthesized covalent TiO₂/O-g-C₃N₄ 2D/2D heterojunction through N-O-Ti covalent bonding, achieving enhanced visible-light photocatalytic activity comparing to heterojunctions fabricated by other methods. Applied DFT calculation to investigate the bonding at heterojunction interface, and performed thorough characterization of the interface via STEM, HRTEM, XPS, and EELS.

Department of Chemistry, SUSTech

May 2017 - Mar 2018

Advisor: Prof. Li Dang

Undergraduate Researcher

- Applied DFT calculation to study the substituent effects on electrocatalytic HER using nickel bis(dithiolene) complexes. Developed an electrocatalytic activity descriptor based on pK_a of dithiolene ligands.

PUBLICATIONS

Total citations: 656; h-index: 8 (Google Scholar Statistics, updated Jun 2021)

1. **Zhang, Z.**; Wang, Y-G.* *Designing Single-Atom Catalysts and Beyond: Advances, Challenges, and Perspectives*. **2021**, submitted
2. **Zhang, Z.**; Wang, Y-G.* *Molecular Design of Nickel Phthalocyanine@Nanocarbon Hybrid Single-atom Catalyst for Active and Stable Electroreduction of CO₂*. **2021**, The Journal of Physical Chemistry C, accepted. DOI: 10.1021/acs.jpcc.1c02508 (**Invited for the special issue: Energy and Catalysis in China**)
3. Wang, Y.¹; **Zhang, Z.**¹; 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*. **2021**, CCS Chemistry, 585-593
4. **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*. **2020**, ACS Catalysis, 10, 23, 13867-13877.
5. Zhang, X.¹; Wang, Y.¹; Gu M.¹; Wang, M.¹; **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 CO₂ Reduction*. **2020**, Nature Energy, 5, 684-692.
6. Venegas, J.¹; **Zhang, Z.**¹; Agbi, T.; McDermott, W.; Alexandrova, A. N.*; Hermans, I.* *Why Boron Nitride is such a Selective Catalyst for the Oxidative Dehydrogenation of Propane*. **2020**, Angewandte Chemie International Edition, 59, 38, 16527-16535. (**VIP paper**)
7. **Zhang, Z.**; Zandkarimi, B.; Alexandrova, A. N.* *Ensembles of metastable states govern heterogeneous catalysis on dynamic interfaces*. **2020**, Accounts of Chemical Research, 53, 2, 447-458.
8. 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*. **2019**, ACS Catalysis, 9, 7, 6252-6261.
9. **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*. **2019**, The Journal of Physical Chemistry Letters, 10, 20-25.

10. Zhong, R.; **Zhang, Z.**; Luo, S.; Zhang, Z. C.; Huang, L.*; Gu, M.* *Comparison of TiO₂ and g-C₃N₄ 2D/2D Nanocomposites from Three Synthesis Protocols for Visible-light Induced Hydrogen Evolution*. **2019**, Catalysis Science & Technology, 9, 75-85 (**Front cover highlight**)
11. **Zhang, Z.**; Yang, T.; Qin, P.; Dang, L.* *Nickel Bis(dithiolene) Complexes for Electrocatalytic Hydrogen Evolution: A Computational Study*. **2018**, Journal of Organometallic Chemistry, 864, 143-147. (**Invited for the special issue: Modern Computational Organometallic Chemistry**)
12. Zhong, R.¹; **Zhang, Z.**¹; Yi, H.; Zeng, L.; Tang, C.; Huang, L.*; Gu, M.* *Covalently Bonded 2D/2D O-g-C₃N₄/TiO₂ Heterojunction for Enhanced Visible-Light Photocatalytic Hydrogen Evolution*. **2018**, Applied Catalysis B: Environmental, 237, 1130-1138.
13. 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 CO₂ Reduction Electrocatalysts Based on Cobalt Phthalocyanine/carbon Nanotube Hybrid Structures*. **2017**, Nature Communications, 8, 14675.

PRESENTATIONS

1. **Zhang, Z.**; Alexandrova, A. N.* *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. **Zhang, Z.**; Liang, Y.* *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.
3. **Zhang, Z.**; Dang, L.* *Designing High-performance Nickel Bis(substituted-dithiolene) Electrocatalysts for HER - A Computational Study* **2018**, Oral Presentation, ACS Symposium: Innovation in Energy Conversion; Dalian, Liaoning, China; Sep 2017.

SCHOLARSHIPS & AWARDS

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| Edwin W. Pauley Fellowship, UCLA | Feb 2020 |
| Outstanding B.Sc. Thesis Award, SUSTech | Jun 2019 |
| Graduate Dean's Scholar Award, UCLA | Apr 2019 |
| University Fellowship, UCLA | Mar 2019 |
| Selected Best Presentations Award in CSST CHEM & MSE division, UCLA | Sep 2018 |
| Cross-disciplinary Scholar in Science and Technology (CSST) Fellowship, UCLA | Jul 2018 |
| Outstanding Scientific Research Potential Award, Shuren College, SUSTech | May 2018 |
| Merit-Based Undergraduate Scholarship, SUSTech | 2016, 2017, 2018 |

TEACHING

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| Teaching Assistant of Chemistry 17: Chemical Principles, UCLA | Winter 2020 |
| Teaching Assistant of Chemistry 30AL: General Chemistry Lab II, UCLA | Fall 2019 |

PROFESSIONAL SERVICES

Affiliations:

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| Member of American Chemical Society | 2018 - Present |
| Vice Chair of ACS Student Chapter, SUSTech | May 2018 - Jun 2019 |

Academic Division Chair of MRS Student Chapter, SUSTech

May 2018 - Jun 2019

Reviewing Services:

Reviewer of Journal of Physical Chemistry (ACS)

2020 - Present

Campus Services:

Academic Department Member of Student Union of Shuren College, SUSTech

Sep 2015 - Sep 2016