

ZISHENG ZHANG

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EDUCATION

University of California, Los Angeles Ph.D. Student in Theoretical/Computational Chemistry	Sep 2019 - Present GPA 3.84/4.00
Southern University of Science and Technology (SUSTech) Bachelor of Science, Chemistry	Sep 2015 - Jun 2019 GPA 3.87/4.00 (Ranking: 1/75)
University of California, Los Angeles Cross-disciplinary Scholar in Science and Technology (CSST)	Jul 2018 - Sep 2018 GPA 4.00/4.00 (Ranking: 1/101)

RESEARCH EXPERIENCE

Department of Chemistry and Biochemistry, UCLA Advisor: Prof. Anastassia Alexandrova and Prof. Philippe Sautet	Sep 2019 - Present 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 (semiempirical QM and DFT), genetic algorithms and machine learning.• Grand Canonical Genetic Algorithm for minima searching of restructured catalytic interface and adsorbate-covered surfaces. Github repo: GOCIA.	
Department of Chemistry and Biochemistry, UCLA Advisor: Prof. Anastassia Alexandrova	Jun 2018 - Dec 2018 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 Advisor: Prof. Jun Li and Prof. Yang-Gang Wang	Sep 2018 - Jun 2019 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 Advisor: Prof. Yongye Liang	Jun 2016 - Jun 2019 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 Advisor: Prof. Limin Huang and Prof. Meng Gu	May 2017 - Oct 2018 Undergraduate Researcher
<ul style="list-style-type: none">• 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.	

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

PUBLICATIONS

- Zhang, Z.**; Wang, Y-G.* *Molecular Design of Nickel Phthalocyanine@Nanocarbon Hybrid Single-atom Catalyst for Active and Stable Electroreduction of CO₂*. **2021**, submitted
- Zhang, Z.**; Wang, Y-G.* *Designing Single-Atom Catalysts and Beyond: Advances, Challenges, and Perspectives*. **2021**, submitted
- 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**, accepted. DOI: 10.31635/ccschem.021.202000590
- 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, accepted. DOI: 10.1021/acscatal.0c03410
- 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
- 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.
- 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.
- 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.
- 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**, Journal of Physical Chemistry Letters, 10, 20-25.
- 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)
- 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.
- 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.
- 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

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 & SERVICES

Teaching Assistant of Chemistry 17: Chemical Principles, UCLA	Winter 2020
Teaching Assistant of Chemistry 30AL: General Chemistry Lab II, UCLA	Fall 2019
Vice President of ACS Student Chapter, SUSTech	May 2018 - Jun 2019
Academic Department Leader of MRS Student Chapter, SUSTech	May 2018 - Jun 2019
Academic Department Member of Student Union of Shuren College, SUSTech	Sep 2015 - Sep 2016