

# ZISHENG ZHANG

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## EDUCATION

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

## RESEARCH EXPERIENCE

<b>Department of Chemistry and Biochemistry, UCLA</b> Advisor: Prof. Anastassia Alexandrova	Sep 2019 - Present Graduate Student Researcher
<ul style="list-style-type: none"><li>· Mechanistic study of Oxidative Dehydrogenation Reaction on Boride surface based on metastable surface states.</li><li>· Modeling electrocatalysis on FTO supported subnano Pt clusters with global optimization and DFT calculation.</li></ul>	
<b>Department of Chemistry and Biochemistry, UCLA</b> Advisor: Prof. Anastassia Alexandrova	Jun 2018 - Dec 2018 CSST Summer Fellow
<ul style="list-style-type: none"><li>· Modeling the dynamic boride surface in catalytic condition with PSO global optimization techniques, DFT calculation, and ab initio MD. Establishing a grand canonical ensemble to study ensemble-averaged surface free energy and Bader charge.</li></ul>	
<b>Department of Chemistry, SUSTech</b> Advisor: Prof. Jun Li and Prof. Yang-Gang Wang	Sep 2018 - Jun 2019 Undergraduate Researcher
<ul style="list-style-type: none"><li>· 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 CO<sub>2</sub> to CO.</li></ul>	
<b>Department of Material Science and Engineering (MSE), SUSTech</b> Advisor: Prof. Yongye Liang	Jun 2016 - Jun 2019 Undergraduate Researcher
<ul style="list-style-type: none"><li>· 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.</li><li>· Fabricated single-atom catalysts through pyrolysis of ZIF-8 encapsulated metal phthalocyanine for ORR.</li><li>· Designed and synthesized bimetallic Cu/Pd NPs supported on oxidized CNT via an adopted co-strong electrostatic adsorption method, achieving selective CO<sub>2</sub>RR to formic acid in a wide potential range.</li><li>· Synthesized and tested CoPc/CNT hybrids for selective electrocatalytic reduction of CO<sub>2</sub>.</li></ul>	
<b>Department of Chemistry &amp; Department of MSE, SUSTech</b> Advisor: Prof. Limin Huang and Prof. Meng Gu	May 2017 - Oct 2018 Undergraduate Researcher
<ul style="list-style-type: none"><li>· Designed and synthesized covalent TiO<sub>2</sub>/O-g-C<sub>3</sub>N<sub>4</sub> 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.</li></ul>	
<b>Department of Chemistry, SUSTech</b> Advisor: Prof. Li Dang	May 2017 - Mar 2018 Undergraduate Researcher
<ul style="list-style-type: none"><li>· Applied DFT calculation to study the substituent effects on electrocatalytic HER using nickel bis(dithiolene) complexes. Developed an electrocatalytic activity descriptor based on pK<sub>a</sub> of dithiolene ligands.</li></ul>	

## PUBLICATIONS

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1. **Zhang, Z.**; Zandkarimi, B.; Alexandrova, A. N.\* *Ensembles of metastable states govern heterogeneous catalysis on dynamic interfaces*. **2019**, submitted to Accounts of Chemical Research.
2. Wang, Y.; Wang, M.; Jiang, Z.; Wang, Q.; Lucero, M.; Zhang, X.; **Zhang, Z.**; 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.
3. **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.
4. 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*. **2019**, Catalysis Science & Technology, accepted, DOI: 10.1039/C8CY00965A (Front cover highlight)
5. **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.
6. Zhong, R.; **Zhang, Z.(equal contribution)**; 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*. **2018**, Applied Catalysis B: Environmental, 237, 1130-1138.
7. 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*. **2017**, Nature Communications, 8, 14675.

## PRESENTATIONS

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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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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

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Teaching Assistant of Chemistry 30AL: General Chemistry Lab II, UCLA	Sep 2019 - Present
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