

# ZI-SHENG ZHANG

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## EDUCATION

<b>Southern University of Science and Technology (SUSTech)</b> Bachelor of Science, Chemistry (expected)	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>

## PROFESSIONAL EXPERIENCE

<b>Shenzhen HUASUAN Technology Co., Ltd</b> Computational Chemistry Consultant	Nov 2018 - Present Shenzhen, Guangdong, China
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## RESEARCH EXPERIENCE

<b>Department of Chemistry and Biochemistry, UCLA</b> Advisor: Prof. Anastassia Alexandrova	Jun 2018 - Dec 2018 CSST Summer Fellow
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- Applying PSO global optimization combined with DFT calculation to investigate the structure of catalytic boride surface under realistic condition; Establishing a grand canonical ensemble to study ensemble-averaged surface free energy and Bader charge; Exploring structural fluxionality of oxidized boride surface with MD.

<b>Department of Chemistry, SUSTech</b> Advisor: Prof. Jun Li and Prof. Yang-Gang Wang	Sep 2018 - Present Undergraduate Researcher
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- Applying DFT calculations to study the pendant group effects on the catalytic activity and stability of nickel phthalocyanine (NiPc) derivatives for selective electroreduction of CO<sub>2</sub> to CO.
- Modeling realistic electrochemical process from ab initio molecular dynamics.

<b>Department of Material Science and Engineering (MSE), SUSTech</b> Advisor: Prof. Yongye Liang	Jun 2016 - Present Undergraduate Researcher
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- Applying DFT calculations to investigate the molecular engineering of FePc derivatives for oxygen reduction reaction. Constructing FePc/CNT hybrids to enhance electrocatalytic activity and stability.
- Fabricating single-atom catalysts through pyrolysis of ZIF-8 encapsulated metal phthalocyanine for metal-air batteries. Funded by the Student's Platform for Innovation and Entrepreneurship Training Program.
- Designing and synthesizing bimetallic Cu/Pd nanoparticles supported on oxidized CNT via an adopted co-strong electrostatic adsorption (SEA) method. Selective electroreduction of CO<sub>2</sub> to formic acid was achieved in a wide potential range. Poster presentation at Nature Conference: Materials Electrochemistry (Jan. 2018)
- Synthesizing and testing CoPc/CNT hybrids for selective electrocatalytic reduction of CO<sub>2</sub>.

<b>Department of Chemistry &amp; Department of MSE, SUSTech</b> Advisor: Prof. Limin Huang and Prof. Meng Gu	May 2017 - Oct 2018 Undergraduate Researcher
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- Designing and synthesizing 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. Applying DFT calculation to investigate the bonding at heterojunction interface, and performing thorough characterization of the interface via STEM, HRTEM, XPS, and EELS.

<b>Department of Chemistry, SUSTech</b> Advisor: Prof. Li Dang	May 2017 - Mar 2018 Undergraduate Researcher
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- Applying 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. Delivering an oral presentation on ACS publications symposium: Innovation in Energy Conversion (Sept. 2017)

## PUBLICATIONS

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1. 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*. **2018**, submitted.
2. **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.
3. 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)
4. **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.
5. 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.
6. 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.

## SCIENTIFIC SKILLS

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**Experimental:** Nanomaterial Synthesis; XRD; TGA; DSC; BET; FL & PL spectroscopy; FT-IR; UV-vis DRS; NMR; SEM; TEM; EDX; GC; HPLC; ICP-MS; Electrochemical & photocatalytic measurements

**Programming & Softwares:** C, JAVA, Python, MatLab, Shell, L<sup>A</sup>T<sub>E</sub>X, SolidWorks, AutoCAD, PhotoShop

**Computational Chemistry:** Gaussian09 & 16, ORCA, MOPAC, Molpro, Material Studio, VASP, Quantum Espresso, CP2K, i-PI, CALYPSO, Molclus, VESTA, Multiwfn, ASE, pymatgen, GaussView, VMD, Jmol

## SCHOLARSHIPS & AWARDS

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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, Shuren College, SUSTech	May 2018
Merit-Based Undergraduate Scholarship, SUSTech	2016, 2017, 2018

## EXTRACURRICULAR ACTIVITIES

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<b>American Chemistry Society (ACS), SUSTech Student Chapter</b> <i>Vice President &amp; Co-founder</i>	May 2018 - Present
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- Organized regular seminars for ACS student members to learn about latest hot papers and discuss interdisciplinary topics in frontiers of chemistry. Invited influential guest speakers to lead forums and seminars.

<b>Material Research Society (MRS), SUSTech Student Chapter</b> <i>Academic Department Leader &amp; Co-founder</i>	May 2018 - Present
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- Organized regular seminars for MRS student members to learn about latest hot papers and conferences.

<b>Student Union of Shuren College, SUSTech</b> <i>Senior Member and Main Contributor, Academic Department</i>	Sep 2015 - Sep 2016
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- Initiated a series of School-wide activities, such as public speaking contests and student-professor meetups.
- Participated in the agenda scheduling, order maintaining and press release.