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EDUCATION

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

SCHOLARSHIPS & AWARDS

Dissertation Year Fellowship, UCLA	Oct 2023
Jim and Barbara Tsay Excellence in Research Award, UCLA	May 2023
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 nd 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

Department of Chemistry and Biochemistry, UCLA	Sep 2019 - Present
Advisor: Prof. Anastassia N. Alexandrova & Prof. Philippe Sautet	Graduate Student Researcher
<ul style="list-style-type: none">• 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.• Grand canonical ensemble representation of fluxional clusters and surfaces in catalytic conditions.• Inverse molecular design of electrochemical CO₂ capturing agents (organic and organometallic) by electronic structure calculation, multi-objective global optimization, and machine learning.• Realistic modeling of electrochemical interface to understand the role of pH, cations, potential, and surface modification in alkaline hydrogen electrocatalysis by explicit solvation and constant potential MD.	
Center for Nanoscale Materials, Argonne National Laboratory	Jun 2022 - Sep 2022
Supervisor: Dr. Maria K. Chan	Research Aide Technical - Ph.D. level
<ul style="list-style-type: none">• Develop an experiment-informed multi-objective global optimizer for crystal structure prediction.	
Department of Chemistry and Biochemistry, UCLA	Jun 2018 - Dec 2018
Supervisor: Prof. Anastassia N. Alexandrova	CSST Summer Fellow
<ul style="list-style-type: none">• Mechanistic study of thermal- and electrocatalysis on borides, focusing on metastable surface states.	

- Dynamics and free energetics of single atom electrocatalysis from *ab initio* MD with explicit electrolyte.
- Molecular design of transition metal phthalocyanine-based catalysts for electrocatalytic CO₂RR and 2/4e⁻ ORR by mechanistic study, high-throughput computation, global optimization, and machine learning.

PUBLICATIONS

Total citations: 1725; h-index: 13 (Google Scholar, Sep 2023); ¹ = co-first authorship; * = corresponding.

Selected^Δ: #31 *JACS*, #29 *Nat. Mater.*, #25 *ACIE*, #21 *JACS*, #20 *Nat. Catal.*, #19 *Chem. Soc. Rev.*, #17 *PNAS*, #8 *ACIE*, #7 *Acc. Chem. Res.*

31. Δ **Zhang, Z.**; Hermans, I.; Alexandrova, A. N.* Off-stoichiometric Restructuring and Sliding Dynamics of Hexagonal Boron Nitride Edges in Conditions of Oxidative Dehydrogenation of Propane. *J. Am. Chem. Soc.*, **2023**, *145*, 17265-17273.
30. Zheng, H.; Li, H.; **Zhang, Z.**; Wang, X.; Jiang, Z.; Tang, Y.; Zhang, J.; Emley, B.; Zhang, Y.; Zhou, H.; Yao, Y.*; Liang, Y.*. Dispersed Nickel Phthalocyanine Molecules on Carbon Nanotubes as Cathode Catalysts for Li-CO₂ Batteries. *small*, **2023**, accepted, DOI: 10.1002/smll.202302768.
29. Δ Wan, C.; **Zhang, Z.**; Dong, J.; Xu, M.; Pu, H.; Baumann, D.; Lin, Z.; Wang, S.; Huang, J.; Shah, A. H.; Pan, X.; Hu, T.; Alexandrova, A. N.*; Huang, Y.*; Duan, X.* Creating a local acidic environment on platinum surface for high-performance hydrogen evolution reaction in alkaline electrolyte. *Nat. Mater.*, **2023**, *22*, 1022-1029.
28. 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.* Electrochemical Carbon Dioxide Capture and Concentration. *Chem. Rev.*, *123*, 8069-8098.
27. Cao, H.; Wang, Q.; **Zhang, Z.**; Yan, H.-M.; Zhao, H.; Yang, H. B.; Liu, B.*; Li, J.; Wang, Y.-G.* Engineering Single-Atom Electrocatalysts for Enhancing Kinetics of Acidic Volmer Reaction. *J. Am. Chem. Soc.*, **2023**, *145*, 13038-13047.
26. Cheng, D.; Wei, Z.; **Zhang, Z.**; Broekmann, P.; Sautet, P.*; Alexandrova, A. N.* Restructuring and Activation of Cu(111) under Electrocatalytic Reduction Conditions. *Angew. Chem., Int. Ed.*, **2023**, *62*, e202218575.
25. Δ **Zhang, Z.**¹; Masubuchi, T.¹; Sautet, P.; Anderson, S. L.*; Alexandrova, A. N.* Hydrogen Evolution on Electrode-Supported Ptn Clusters: Ensemble of Hydride States Governs the Size Dependent Reactivity. *Angew. Chem., Int. Ed.*, **2023**, *62*, e202218210.
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 CO₂ 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. Δ **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. Δ 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. Δ Barlow, J. M.¹; Clarke, L.¹; **Zhang, Z.**¹; Daniel, B.; Leonard, M.; Zito, A.; Brushett, F.*; Alexandrova, A. N.*; Yang, J. Y.* Molecular Design of Redox Carriers for Electrochemical CO₂ 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 CO₂ Electroreduction on Single Nickel Atom Catalyst with Explicit Solvation. *ACS Catal.*, **2022**, *12*, 11380-11390.
17. Δ **Zhang, Z.**; Kummeth, A. L.; Yang, J. Y.*; Alexandrova, A. N.* Inverse Molecular Design of Alkoxides and Phenoxides for Aqueous Direct Air Capture of CO₂. *Proc. Nat. Acad. Sci.*, **2022**, *119*, e2123496119
16. Cao, H.¹; **Zhang, Z.**¹; Chen, J. W.; Wang, Y.-G.* Potential Dependent Free Energy Relationship in Interpreting the Electrochemical Performance of CO₂ Reduction on Single Atom Catalyst. *ACS Catal.*, **2022**, *12*, 6606-6617.
15. Chen, J.W.¹; **Zhang, Z.**¹; Yan, H.¹; 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.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. *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 CO₂. *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.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. *Nat. Energy*, **2020**, *5*, 684-692.
8. Δ 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. *Angew. Chem., Int.*

Ed., **2020**, 59, 16527-16535.

- Designated as a "Very Important Paper (VIP)" article by evaluators

7. **Δ 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 TiO₂ and g-C₃N₄ 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.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. *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 CO₂ Reduction Electrocatalysts Based on Cobalt Phthalocyanine/carbon Nanotube Hybrid Structures. *Nat. Commun.* **2017**, 8, 14675.

PRESENTATIONS

10. "Unriddling the cationic and pH effect in alkaline hydrogen evolution reaction on Pt" Oral Presentation, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.
9. "Inverse molecular design of alkoxides and phenoxides for aqueous direct air capture of CO₂" Oral Presentation, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.
8. "Modeling fluxionality and off-stoichiometric restructuring at electrochemical interfaces." Poster Presentations, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.
- ACS COMP - CCG Excellence in Research Award Symposium
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 CO₂ Capture." Oral Presentation, *Sloan Annual Meeting: CO₂ 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 Electrorreduction 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

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

Shawn Chiu, Ph.D. Student (Chemistry), UCLA	2022 - Present
Samuel Greenbank, Undergraduate (visiting), UCLA	2022 - 2023
Robert Lavroff, Ph.D. Student (Chemistry), UCLA	2021 - Present
Winston Gee, Ph.D. Student (Chemistry), UCLA	2021 - Present
Edison Cummings, Undergraduate (Chemistry), UCLA	2022 - Present
Jennifer Tjia, Undergraduate (Chemistry), UCLA	2022 - 2023
Tom Z. Hong, Undergraduate (Mathematics), UCLA	2022 - 2023

PROFESSIONAL SERVICES

Affiliations:

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

Reviewing Services:

(33 completed journal reviews, Web of Science Statistics, updated Sep 2023)

Reviewer of GenBio@NeurIPS	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