Zisheng Zhang · (張 孜晟)

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Academic Appointments

2026 **Stanford University** — Stanford, California
Assistant Professor (Prospective) in Chemical Engineering

Education & Training

2026 **SLAC National Accelerator Laboratory** — Menlo Park, California
Stanford Energy Fellow Host: Dr. Frank Abild-Pedersen

2024 **University of California, Los Angeles** (UCLA) — Los Angeles, California
Ph. D. in Chemistry. Advisor: Prof. Anastassia N. Alexandrova

2022 **Argonne National Laboratory** — Lemont, Illinois
CNM Graduate Research Aide. Advisor: Dr. Maria K. Chan

2021 **University of California, Los Angeles** — Los Angeles, California
M. Sc. in Chemistry. Advisor: Prof. Anastassia N. Alexandrova

2019 **South University of Science and Technology of China** (SUSTC) — Shenzhen, Canton
B. Sc. in Chemistry. Advisor: Prof. Jun Li (李 隽)

2018 **University of California, Los Angeles** — Los Angeles, California
CSST Undergraduate Fellow. Advisor: Prof. Anastassia N. Alexandrova

Publications

Total citations: 4,947 | *h*-index: 32 | *i*10-index: 43 (Apr 2026) [1] = co-first; *= corresponding.

52. Xin, H.; Kitchin, J. R.; López, N.; Schweitzer, N. M.; Abolhasani, M.; Artrith, N.; Árnadóttir, L.; Choudhary, K.; Ding, R.; Frenkel, A. I.; Gauthier, J. A.; Goldsmith, B. R.; Farimani, A. B.; Grabow, L. C.; Gunasooriya, G. T. K. K.; Hu, G.; Josephson, T. R.; Kulik, H. J.; Kumar, R.; Laino, T.; Li, H.; Li, X.-Y.; Li, W.; Linic, S.; Liu, C.; Liu, C.; Liu, F.; Liu, M.; Ma, P.; Medford, A. J.; Mukhopadhyay, S.; Ou, P.; Paolucci, C.; Peng, J.; Phillips, C.; Porosoff, M. D.; Qi, L.; Rosen, A. S.; Sun, S.; Szilvási, T.; Voss, J.; Wang, S.; Wang, X.; Winther, K.; Wu, Q.; Zhang, D.; **Zhang, Z.** Transparent Reporting for Agentic Catalysis Enabled by Artificial Intelligence (TRACE-AI): Community Guidelines and a Publication Checklist. Chem Catal., **2026**, accepted, DOI: 10.26434/chemrxiv.15001239/v1.

51. Raciti, D.*; **Zhang, Z.***; Guo, A.; Moffat, T. P.*. O2 Reduction Stimulates Adatom Generation on Cu (111) Catalyzing Hydrogen Evolution. J. Am. Chem. Soc., **2026**, *148*, 7401–7414.

50. **Zhang, Z.**; Abild-Pedersen, F.*. Dopant-Dependent Boron Arrangement and Chemistry of Metal Boride Surface. ACS Catal., **2026**, accepted, DOI: 10.1021/acscatal.5c08265.

49. **Zhang, Z.***; Zhou, X. Non-Equilibrium Restructurings in Catalysis: A Chemical Space Odyssey. MRS Commun., **2025**, DOI: 10.1557/s43579-025-00902-x.
- Invited, Early Career Distinguished Presenter Prospective (2025 MRS Spring).

48. **Zhang, Z.**; Abild-Pedersen, F.*. Unlocking Switchable Reactivity of MBene via Asymmetric Surface Adsorption. J. Phys. Chem. Lett., **2025**, *16*, 12619–12624.

47. Wei, J.; **Zhang, Z.**; Gee, W.; Zhou, Y.-W.; Herran, M.; Sautet, P.; Alexandrova, A. N.; Cuenya, B. R.; Kley, C. S. The role of surface hydroxyls in atomic-scale copper re-structuring during CO electroreduction. J. Am. Chem. Soc., **2025**, *147*, 45178–45188.

46. Yin, B.; Wang, J.; Du, W.; Wang, P.; Ying, P.; Jia, H.; **Zhang, Z.**; Du, Y.; Gomes, C. P.; Henkelman, G.; Duan, C.; Xiao, H. AlphaNet: Scaling Up Local Frame-based Atomistic Interatomic Potential. npj Comp. Mater., **2025**, *11*, 332.

45. Choi, J.; Banerjee, A.; Ross, R. D.; **Zhang, Z.**; Chiu, S.; Sacci, R. L.; Veith, G. M.; Hahn, C.; Alexandrova, A. N.*; Morales-Guio, C. G.*. Amine Structure Governs Corrosion Rates of Copper Catalysts in Electrochemical Reactive Capture of CO_2. J. Phys. Chem. C, **2025**, *129*, 16009–16019.

44. **Zhang, Z.**; Abild-Pedersen, F.*. Off-Equilibrium Reactivity of Boron-Enriched Metal Diboride Surface in Electroreduction Condition. ACS Catal., **2025**, *15*, 12340–12350.

43. Li, G.; Chiu, S.; Morgan, H. W. T.; Fuchs, A. T.; Isakov, A.; Poths, P.; **Zhang, Z.**; Alexandrova, A. N.*; Anderson, S. L.*. Size-Dependent Effects of Ge Addition on the Coking and Sintering Tendency of Pt_nGe_m/Alumina (n = 4, 7, 11) Model Catalysts. J. Catal., **2025**, *448*, 116196.

42. Cheng, D.; Nguyen, K.-L. C.; Sumaria, V.; Wei, Z.; **Zhang, Z.**; Gee, W.; Li, Y.; Morales-Guio, C. G.; Heyde, M.; Roldan Cuenya, B.; Alexandrova, A. N.*; Sautet, P.*. Structure Sensitivity and Catalyst Restructuring for CO_2 Electro-reduction on Copper. Nat. Commun., **2025**, *16*, 4064.

41. Wan, C.; **Zhang, Z.**; Wang, S.; Sun, Q.; Liu, E.; Pu, H.; Zhang, A.; Chen, Z.; Shah, A. H.; Fu, X.; Alexandrova, A. N.; Jia, Q.; Huang, Y.*; Duan, X.*. Reorganizing the Pt Surface Water Structure for Highly Efficient Alkaline Hydrogen Oxidation Reaction. J. Am. Chem. Soc., **2025**, *147*, 12162–12169.

40. **Zhang, Z.***; Gee, W.; Lavroff, R. H.; Alexandrova, A. N.*. GOCIA: grand canonical Global Optimizer for Clusters, Interfaces, and Adsorbates. PCCP, **2025**, *27*, 696–706.

39. Lavroff, R. H.; Cummings, E.; Sawant, K.; **Zhang, Z.**; Sautet, P.*; Alexandrova, A. N.*. Cu-supported ZnO in Conditions of CO_2 Reduction to Methanol: Why 0.2 ML Coverage? J. Phys. Chem. Lett., **2024**, *15*, 11745–11752.

38. **Zhang, Z.**; Gee, W.; Sautet, P.*; Alexandrova, A. N.*. H and CO Co-induced Adatom Formation on Cu in CO_2 Electroreduction Conditions. J. Am. Chem. Soc., **2024**, *146*, 16119–16127.

37. Qie, B.; Wang, Z.; Jiang, J.; **Zhang, Z.**; Jacobse, P. H.; Lu, J.; Li, X.; Liu, F.; Alexandrova, A. N.; Louie, S. G.*; Crommie, M. F.*; Fischer, F. R.*. Low Dimensional N-Heterocyclic Carbene-Metal Lattices. Science, **2024**, *384*, 895–901.

36. Shah, A. H.[1]; **Zhang, Z.[1]**; Wan, C.; Wang, S.; Zhang, A.; Wang, L.; Alexandrova, A. N.*; Huang, Y.*; Duan, X.*. The platinum-surface water orientation dictates hydrogen evolution reaction kinetics in alkaline media. J. Am. Chem. Soc., **2024**, *146*, 9623–9630.

35. Yan, H.-M.; **Zhang, Z.**; Wang, Y.-G.*. Coverage-Induced Cation Dehydration and Migration for Enhanced CO–CO Coupling on Cu Electrocatalysts. ACS Catal., **2024**, *14*, 3596–3605.

34. **Zhang, Z.**; Li, J.; Wang, Y.-G.*. Modeling Interfacial Dynamics on Single Atom Electrocatalysts: Explicit Solvation and Potential Dependence. Acc. Chem. Res., **2024**, *57*, 198–207.

33. Cendejas, M.; Mellone, O. A. P.; Unni, K.; **Zhang, Z.**; Jacob, J.; Ibrahim, F.; Dong, S.; Vinson, J.; Alexandrova, A. N.; Sokaras, D.*; Bare, S. R.*; Hermans, I.*. Tracking Active Phase Behavior on Boron Nitride during the Oxidative Dehydrogenation of Propane Using Operando X-Ray Raman Spectroscopy. J. Am. Chem. Soc., **2023**, *145*, 25686–25694.

32. Yu, Y.[1]; Koh, H.[1]; **Zhang, Z.[1]**; Yang, Z.; Alexandrova, A. N.; Stach, E. A.*; Xie, J.*. Kinetic Pathways of Fast Lithium Transport in Solid Electrolyte Interphases with Discrete Inorganic Components. Energy Environ. Sci., **2023**, *16*, 5904–5915.

31. **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**, *19*, 2302768.

29. 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., **2023**, *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. **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 CO_2 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. **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. Shah, A. H.; **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. 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 CO_2 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 CO_2 Electroreduction on Single Nickel Atom Catalyst with Explicit Solvation. ACS Catal., **2022**, *12*, 11380–11390.

17. **Zhang, Z.**; Kummeth, A. L.; Yang, J. Y.*; Alexandrova, A. N.*. Inverse Molecular Design of Alkoxides and Phenoxides for Aqueous Direct Air Capture of CO_2. 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 CO_2 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 CO_2. 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 CO_2 Reduction. Nat. Energy, **2020**, *5*, 684–692.

8. 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. **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 TiO_2 and g-C_3N_4 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-C_3N_4/TiO_2 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., **2018**, *864*, 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 CO_2 Reduction Electrocatalysts Based on Cobalt Phthalocyanine/carbon Nanotube Hybrid Structures. Nat. Commun., **2017**, *8*, 14675.

?. McKeown-Green, A. S.; Moradifar, P.; **Zhang, Z.**; Lim, C.; Barnum, A.; Yuan, L.; Sinclair, R.; Abild-Pedersen, F.; Ophus, C.; Dionne, J. A.*. Ammonia Catalyst Evolution Under Reactor Conditions Revealed by Environmental and Multimodal Electron Microscopy. Under review, **2026**, preprint: 10.48550/arXiv.2602.00433.

?. Goswani, A.; **Zhang, Z.**; Alexandrova, A. N.*. CO2 Electroreduction on Borated Copper Surfaces: Boron Active Sites, not Copper. Under review, **2025**, preprint: 10.26434/chemrxiv-2025-0ngnn.

Presentations (since 2020)

38. "Grand Canonical Modeling of Catalyst Reconstruction in and out of Equilibrium" Talk, *SUNCAT Theory Seminar*, Menlo Park, CA, Dec 2025.

37. "Designing Metal Boride Electrocatalysts" Poster Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

36. "Understanding Catalyst (de)Activation with AI-Accelerated Statistical Sampling" Poster Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

35. "Unlocking Switchable Reactivity of 2D Boride By Asymmetric Adsorption" Oral Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

34. "Dopant-Dependent Arrangement and Chemistry of Surface B on Metal Diborides" Oral Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

33. ”Gocia: A Grand Canonical Global Optimizer for Clusters, Interfaces, and Adsorbates” Oral Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

32. ”Exploring Non-Equilibrium Chemical Subspace in Electrocatalysis” Oral Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

31. ”Off-Equilibrium Reactivity of B-Enriched Metal Diboride in Electro-Reduction Conditions” Oral Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

30. ”Modeling Constant-Potential Dynamics and Free Energetics of Electrochemical Interfaces” Oral Presentation, *AIChE 2025 Meeting*, Boston, MA, Nov 2025.

29. ”Exploring Reconstructed Boride Surfaces for Electrocatalysis.” Poster presentation, *2025 SUNCAT Summer Institute*, Menlo Park, CA, Aug 2025.

28. ”Hexagonal Boron Nitride Surfaces Under Condition of Oxidative Dehydrogenation of Propane – Off-stoichiometric Restructuring and Metastable Active Species”, Oral presentation, *2025 MRS Spring Meeting*, Seattle, WA, Apr 2025.

27. ”Grand Canonical Modeling of Adsorbate-Induced Restructuring of Cu Electrode”, Oral presentation, *2025 MRS Spring Meeting*, Seattle, WA, Apr 2025.

26. ”Reactivity and structural evolution of B-rich metal diboride in acidic electroreduction conditions”, Oral presentation, *2025 APS Global Summit*, Anaheim, CA, Mar 2025.

25. ”Grand Canonical Approach to Modeling Catalysts Restructuring” Poster Presentation, Oral presentation, *2025 APS GERA Energy Workshop*, Anaheim, CA, Mar 2025.

24. ”Grand Canonical Approach to Modeling Catalysts Restructuring” Talk, *SUNCAT Theory Seminar*, Menlo Park, CA, Dec 2024.

23. ”Grand Canonical Approach to Modeling Dynamic Catalysts” Invited Talk, *Digital Catalysis Workshop*, Online Seminar, Dec 2024.

22. ”Unriddling the Cationic and pH Effect in Alkaline Hydrogen Evolution Reaction on Pt” Oral Presentation, *AIChE 2024 Meeting*, San Diego, CA, Oct 2024.

21. ”Grand Canonical Approach to Modeling Dynamic Catalysts: From Thermal to Electro-Catalysis, from Clusters to Surfaces” Oral Presentation, *AIChE 2024 Meeting*, San Diego, CA, Oct 2024.

20. ”Modeling Interfacial Dynamics on Single Atom Electrocatalysts: Explicit Solvation and Potential Dependence” Oral Presentation, *AIChE 2024 Meeting*, San Diego, CA, Oct 2024.

19. ”Modeling Adsorbate-Induced Restructuring of Cu Surface in Electro-Reduction Conditions” Oral Presentation, *AIChE 2024 Meeting*, San Diego, CA, Oct 2024.

18. ”Multi-Objective Inverse Molecular Design of CO2 Capturing Agents” Oral Presentation, *AIChE 2024 Meeting*, San Diego, CA, Oct 2024.

17. ”Hexagonal Boron Nitride Surfaces Under Condition of Oxidative Dehydrogenation of Propane: Off-Stoichiometric Restructuring and Metastable Active Species” Oral Presentation, *AIChE 2024 Meeting*, San Diego, CA, Oct 2024.

16. ”Grand Canonical Representation of Dynamic Electrocatalysts: From Clusters to Surfaces” Poster Presentation, *AI for Multidisciplinary Exploration and Discovery (AIMED) Workshop on Heterogeneous Catalysis*, Chicago, IL, Oct 2024.

15. ”Grand Canonical Approach to Modeling Dynamic Catalysts: From Thermal to Electro, From Clusters to Surfaces” Invited Talk, *Invited Online Seminar*; Institute of Energy and Climate Research, Forschungszentrum Jülich, Sep 2024.

14. ”Adsorbate-Induced Restructuring of Copper Electrodes in Electroreduction Conditions” Oral Presentation, *18th ICC – International Congress on Catalysis*; Lyon, France; Jul 2024.

13. ”Grand Canonical Representation of Dynamic Electrocatalysts: From Clusters to Surfaces” Poster Presentation, *18th ICC – International Congress on Catalysis*; Lyon, France; Jul 2024.

12. ”Grand Canonical Approach to Modeling Dynamic Catalysts from thermal to electro-, from clusters to surfaces” Invited Talk, *Laboratoire de Chemie, ENS Lyon*; Lyon, France; Jul 2024.

11. ”Grand Canonical Approach to Modeling Electrochemical Restructuring of Cu Surface” Invited Talk, *South East Hub TheMoSia Meeting, ISA*; Lyon, France; Jul 2024.

10. ”Grand Canonical Approach to Modeling Dynamic Catalysts: From Thermal to Electro, From Clusters to Surfaces” Invited Talk, *Chemical Engineering Faculty Search Seminar*; Stanford, CA, United States; Mar, 2024.

9. ”Grand Canonical Ensemble Representation of Dynamic Catalysts: From Thermal to Electro, From Clusters to Surfaces” Invited Talk, *Liu Group Seminar*; Austin, TX, United States; Feb, 2024.

8. ”Grand Canonical Ensemble Representation of Dynamic Catalysts: From Thermal to Electro-catalysis, From Clusters to Surfaces” Dissertation Talk, *Exit Seminar*; Los Angeles, CA, United States; Nov 2023.

7. ”Unriddling the cationic and pH effect in alkaline hydrogen evolution reaction on Pt” Oral Presentation, *ACS Spring 2023*; Indianapolis, IN, United States; Mar 2023.

6. ”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.

5. ”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

4. ”Modeling Fluxionality and Off-Stoichiometric Restructuring at Electrochemical Interfaces.” Virtual Poster Presentation, *#RSCPoster Twitter Conference*; link; Mar 2023.

3. ”Modeling Catalysis the Hard Way: Grand Canonical Ensemble Representation of Catalytic Interfaces.” Invited Talk, *Henkelman Group Seminar*; Austin, TX, United states; Oct 2022.

2. ”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

1. ”Inverse Molecular Design of Alkoxide and Phenoxide for Aqueous CO_2 Capture.” Oral Presentation, *Sloan Annual Meeting: CO_2 capture*; Irvine, CA, United States; Mar 2022.

GRANTS & COMPUTATIONAL RESOURCES

Lead, OCLF Frontier Allocation	2026
Contributor, DOE SUNCAT-FWP	2025
Contributor, DOE BES	2020-2024
Contributor, NSF CBET	2020-2024
Contributor, DOE NERSC allocation	2019-2025
Contributor, DOE INCITE allocation	2020-2024
Contributor, NSF ACCESS allocation	2020-2024

SCHOLARSHIPS / FELLOWSHIPS / AWARDS

Early Career Distinguished Presenter, MRS	Mar, 2025
2025 GERA Energy Workshop Best Poster Award, APS	Mar, 2025
2025 GERA Energy Workshop Travel Award, APS	Dec, 2024
Faraday Horison Prize, RSC	2024
Evelyn Pan Dissertation Award, UCLA	Apr, 2024
Stanford Energy Postdoctoral Fellowship, Stanford University	Jan, 2024
18th International Congress on Catalysis (Lyon, France) Young Researcher Support, IACS	Mar 2024
18th International Congress on Catalysis (Lyon, France) Travel Award, NACS	Mar 2024
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 2nd Year Research and Academics Award, UCLA	May 2022
Edwin W. Pauley Fellowship, UCLA	Feb 2020
Outstanding B.Sc. Thesis Award, SUSTC	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, SUSTC	2016, 2017, 2018

TEACHING & OUTREACH

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

Graduate Students: Jinwen Liu (Leiden University, Chemistry), Hengyue Xu (Tsinghua University, Chemistry), Anubhav Goswami (UCLA, Chemistry), Shawn Chiu (UCLA, Chemistry), Robert Lavroff (UCLA, Chemistry), Winston Gee (UCLA, Chemistry), Dongfang Cheng (UCLA, Chemical Engineering)

Undergraduate Students: Dylan Karkainen (UCLA, Chemistry), Jack Cokas (UCLA, Chemistry), Samuel Greenbank (Uni of Manchester, Visiting), Edison Cummings (UCLA, Chemistry), Jennifer Tjia (UCLA, Chemistry), Tom Z. Hong (UCLA, Chemistry), Shuqi Luo (SUSTC, Chemistry)

Subgroups: Leader of the Dynamic Electrocatalysis subgroup @Alexandrova Lab

PROFESSIONAL SERVICES

Peer Review (98 completed journal reviews, Web of Science Statistics, updated Mar 2026):
Journals: *National Science Review, Accounts of Chemical Research, Advanced Materials, Journal of Catalysis, One Earth, Molecular Catalysis, Molecular Systems Design & Engineering, Reactions, The Journal of Chemical Physics, ChemSusChem, ACS Applied Materials & Interfaces, npj Computational Materials, Journal of Chemical Physics, Journal of the American Chemical Society, JACS Au, The New Journal of Chemistry, The Journal of Physical Chemistry C, Computational and Theoretical Chemistry*
Conference: *International Conference on Machine Learning, Conference on Neural Information Processing Systems*
Book: *ACS In Focus series*

Editorial:

Catalyst — Guest editor of Special Issue: Predictive Modeling in Catalysis	2025

Academic Society:

Materials Research Society	2024 - Present
American Physical Society	2024 - Present
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

Session Chairing:

MT05.04 Sciences in Nanocrystal Syntheses and Properties	2025 MRS Spring Meeting
MAR-W49 Advances in Modeling Phonon, Spin, Charge, and Chemical Dynamics	2025 APS Global Summit