

Stanford



Zisheng Zhang

Postdoctoral Scholar, Photon Science, SLAC

 Curriculum Vitae available Online

Bio

BIO

Zisheng Zhang is an incoming Assistant Professor of Chemical Engineering, starting in Fall 2026. He is currently a Stanford Energy Fellow at SUNCAT Center for Interface Science and Catalysis, co-hosted by Dr. Frank Abild-Pedersen (SLAC) and Prof. Thomas Jaramillo (Chemical Engineering). He is interested in physics-steered, complexity-driven, and AI-accelerated simulations for understanding, design, and discovery of novel functional catalysts, materials, molecules, and interfaces.

ZZ grew up in Wuhan and received undergraduate training in both experimental and computational chemistry at South University of Science and Technology of China (with Prof. Jun Li) and University of California, Los Angeles (with Prof. Anastassia N. Alexandrova). He then stayed at UCLA and obtained his M.Sc. and Ph.D. in Theoretical and Computational Chemistry. During PhD study, he did research internship at Argonne National Lab in 2022 with Dr. Maria Chan.

STANFORD ADVISORS

- Frank Abild-Pedersen, Postdoctoral Research Mentor
- Thomas Jaramillo, Postdoctoral Faculty Sponsor

LINKS

- Google Scholar: https://scholar.google.com/citations?user=oYBJT_kAAAAJ&hl=en

Research & Scholarship

LAB AFFILIATIONS

- Frank Abild-Pedersen, SUNCAT Theory (9/1/2024)

Publications

PUBLICATIONS

- **O₂ Reduction Stimulates Adatom Generation on Cu(111) Catalyzing Hydrogen Evolution.** *Journal of the American Chemical Society*
Raciti, D., Zhang, Z., Guo, A., Moffat, T. P.
2026
- **Dopant-Dependent Boron Arrangement and Chemistry of Metal Boride Surface** *ACS CATALYSIS*
Zhang, Z., Abild-Pedersen, F.
2026

- **Non-equilibrium restructurings in catalysis: A chemical space odyssey** *MRS COMMUNICATIONS*
Zhang, Z., Zhou, X.
2025
- **Unlocking Switchable Reactivity of MBene via Asymmetric Surface Adsorption.** *The journal of physical chemistry letters*
Zhang, Z., Abild-Pedersen, F.
2025: 12619-12624
- **Role of Surface Hydroxyls in Atomic-Scale Copper Restructuring during CO Electroreduction.** *Journal of the American Chemical Society*
Wei, J., Zhang, Z., Gee, W., Wei, Y., Zhou, Y., Herran, M., Sautet, P., Alexandrova, A. N., Roldan Cuenya, B., Kley, C. S.
2025
- **AlphaNet: scaling up local-frame-based neural network interatomic potentials** *NPJ COMPUTATIONAL MATERIALS*
Yin, B., Wang, J., Du, W., Wang, P., Ying, P., Jia, H., Zhang, Z., Du, Y., Gomes, C., Duan, C., Henkelman, G., Xiao, H.
2025; 11 (1)
- **Off-Equilibrium Reactivity of Boron-Enriched Metal Diboride Surfaces in Electroreduction Conditions** *ACS CATALYSIS*
Zhang, Z., Abild-Pedersen, F.
2025
- **Structure Sensitivity and Catalyst Restructuring for CO₂ Electro-reduction on Copper** *NATURE COMMUNICATIONS*
Cheng, D., Nguyen, K. 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.
2025; 16 (1): 4064
- **Reorganizing the Pt Surface Water Structure for Highly Efficient Alkaline Hydrogen Oxidation Reaction.** *Journal of the American Chemical Society*
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, et al
2025
- **GOCIA: a grand canonical global optimizer for clusters, interfaces, and adsorbates.** *Physical chemistry chemical physics : PCCP*
Zhang, Z., Gee, W., Lavroff, R. H., Alexandrova, A. N.
2024
- **Cu-Supported ZnO under Conditions of CO₂ Reduction to Methanol: Why 0.2 ML Coverage?** *The journal of physical chemistry letters*
Lavroff, R. H., Cummings, E., Sawant, K., Zhang, Z., Sautet, P., Alexandrova, A. N.
2024: 11745-11752
- **Synthesis and characterization of low-dimensional N-heterocyclic carbene lattices** *SCIENCE*
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.
2024; 384 (6698): 895-901
- **Tracking Active Phase Behavior on Boron Nitride during the Oxidative Dehydrogenation of Propane Using Operando X-ray Raman Spectroscopy.** *Journal of the American Chemical Society*
Cendejas, M. C., Paredes Mellone, O. A., Kurumbail, U., Zhang, Z., Jansen, J. H., Ibrahim, F., Dong, S., Vinson, J., Alexandrova, A. N., Sokaras, D., Bare, S. R., Hermans, I.
2023
- **Molecular engineering of dispersed nickel phthalocyanines on carbon nanotubes for selective CO₂ reduction** *NATURE ENERGY*
Zhang, X., Wang, Y., Gu, M., Wang, M., Zhang, Z., Pan, W., Jiang, Z., Zheng, H., Lucero, M., Wang, H., Sterbinsky, G. E., Ma, Q., Wang, et al
2020