

Xinzhe Yang • 杨欣哲

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EDUCATION

- ♦ **Peking University** Sep 2022 – Jun 2025 (expected)
M.S. in Materials Physics and Chemistry Advisor: Prof. Feng Pan
- ♦ **Xiamen University** Sep 2018 – Jun 2022
B.S. in Chemistry (GPA: 3.60/4.00, top 10%) Advisor: Prof. Jun Cheng

RESEARCH EXPERIENCE

- ♦ **Graduate Student Researcher**, Advisor: Feng Pan Sep 2022 – Present
School of Advanced Materials, Peking University, Shenzhen Graduate School
 - Employ AIMD simulations with enhanced sampling to investigate cation effects in electrocatalytic reactions: reveal a comprehensive atomic mechanism related to electrochemical CO₂RR selectivity; decipher the importance of *H regulatory strategy to enhance NO₃RR
 - Explore complex reaction network using a graph based theoretical approach for electrochemical C-N coupling on single-atom catalysts
- ♦ **Research Intern**, Advisor: Wanlu Li Apr 2024 – Present (remote)
Department of Chemical and Nano Engineering, University of California, San Diego
 - Evaluate the impact of cation on hydrophobic hydration in the electric double layer from AIMD trajectories, and investigate their modulation of the energy profiles of electrochemical processes
- ♦ **Undergraduate Researcher**, Advisor: Jun Cheng Jun 2021 – Jun 2022
College of Chemistry and Chemical Engineering, Xiamen University
 - Develop automated workflows to construct metal-water interfaces for efficient chemical modeling, and incorporate them for accelerating MD simulations through machine learning potentials

PUBLICATIONS

4. Junjie Pan#, Haowen Ding#, **Xinzhe Yang#**, Xianhui Liang, Shanglin Wu, Mingzheng Zhang, Shunning Li*, Shisheng Zheng*, Feng Pan*. Autonomous Exploration of Reaction Pathways for Electrochemical C-N Coupling on Single-Atom Catalysts. (Manuscript submitted)
3. Shisheng Zheng*, **Xinzhe Yang**, Zhong-Zhang Shi, Haowen Ding, Feng Pan*, Jian-Feng Li*. The Loss of Interfacial Water-Adsorbate Hydrogen Bond Connectivity Positions Surface-Active Hydrogen as a Crucial Intermediate to Enhance Nitrate Reduction Reaction. *J. Am. Chem. Soc.* (In revision)
2. Haowen Ding, Shisheng Zheng*, **Xinzhe Yang**, Junjie Pan, Zhefeng Chen, Mingzheng Zhang, Shunning Li*, Feng Pan*. The Role of Surface Hydrogen Coverage in C–C Coupling Process for CO₂ Electroreduction on Ni-Based Catalysts. *ACS Catal.* (In revision)
1. **Xinzhe Yang**, Haowen Ding, Shunning Li, Shisheng Zheng*, Jian-Feng Li, Feng Pan*. Cation-Induced Interfacial Hydrophobic Microenvironment Promotes the C–C Coupling in Electrochemical CO₂ Reduction. *J. Am. Chem. Soc.* 2024, 146, 8, 5532–5542.

ACADEMIC ACTIVITIES

- ♦ Poster Presentation, **the 34th Chinese Chemical Society Congress**, Guangzhou, China Jun 2024

SKILLS

Software: VASP, CP2K, LAMMPS

Programming: Python, C/C++, Fortran, Bash