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

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. 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 Press

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 Press

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.

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 CO_2RR selectivity; decipher the importance of *H regulatory strategy to enhance NO_3RR
  - 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

ACADEMIC ACTIVITIES

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

SKILLS

Software: VASP, CP2K, LAMMPS

Programming: Python, C/C++, Bash