Xinzhe Yang • 杨欣哲

Email: xinzheyang@stu.pku.edu.cn; **Website**: xzyang99.github.io

EDUCATION

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

RESEARCH EXPERIENCE

- **Graduate Student Researcher, Feng Pan Group** 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
  - Observe a correlation between the water-adsorbate stabilization effect and the alleviation in free energy
  - Reveal a comprehensive atomic mechanism of the cation–water–adsorbate interactions related to electrochemical CO_2RR selectivity
  - Decipher the role of cation in understanding the *H regulatory strategy in electrochemical NO_3RR
  - Resolve contrasting trends of cation-dependent HER on metal electrodes from a molecular perspective
- **Research Intern, Wanlu Li Group** Apr 2024 – Present (remote)
  Department of NanoEngineering, University of California, San Diego
  Examine the influence of cation on cavity formation energy at electrochemical interfaces
  - Calculate cavity formation energy in the electric double layer from AIMD trajectories
  - Study hydrophobic hydration in modifying energy profiles of electrochemical processes
- **Undergraduate Researcher, Jun Cheng Group** Jun 2021 – Jun 2022
  College of Chemistry and Chemical Engineering, Xiamen University
  Develop automated workflows for efficient chemical modeling
  - Establish an automated workflow for convenient construction of metal-water interfaces
  - Incorporate automated workflows for accelerating MD simulations through machine learning potentials

PUBLICATIONS

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. (Manuscript submitted)

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 CCS Congress**, Guangzhou, Guangdong, China Jun 2024

SKILLS

Software: VASP, CP2K, LAMMPS; **Programming:** Python, C/C++, Fortran