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: 3.59/4.00, top 10%) Advisor: Prof. Jun Cheng

RESEARCH INTEREST

My research primarily focuses on theoretical investigations of electrochemical interfaces, particularly delving into their dynamic properties under realistic reaction conditions. I also have a broad interest in first-principles calculations and molecular dynamics simulations within the realms of chemistry and materials science.

RESEARCH EXPERIENCE

School of Advanced Materials, Peking University, Shenzhen Graduate School

Research Assistant at Prof. Feng Pan's Research Group Sep 2022 –

Research project: Theoretical Study on Cation Effect in Electrocatalysis

College of Chemistry and Chemical Engineering, Xiamen University

Graduation Thesis at Prof. Jun Cheng's Research Group Sep 2021 – Jun 2022

Research project: Automating Workflow for Constructing Metal-Water Interfaces

PUBLICATIONS

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.

SKILLS

- **Software:** VASP, CP2K, LAMMPS
- **Programming:** Python, C++