

Xinzhe Yang • 杨欣哲

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EDUCATION

- ♦ **Peking University** Sep 2022 – Jun 2025 (expected)
M.E. 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

5. 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. *ACS Catal.* Accepted
4. Shisheng Zheng, Haowen Ding, **Xinzhe Yang**, Shunning Li*, Feng Pan*. Automating Discovery of Electrochemical Urea Synthesis Reaction Paths via Active Learning and Graph Theory. *CCS Chem.* Accepted
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.* 2024, 146, 39, 26965-26974
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.* 2024, 14, 19, 14330-14338
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

- ♦ **School of Advanced Materials, Peking University, Shenzhen Graduate School**
Graduate Student Researcher with Prof. Feng Pan Sep 2022 – Present
Investigate cation effects in electrocatalytic reactions using AIMD simulations
 - Reveal a comprehensive cation-water-adsorbate interaction related to CO₂RR selectivity: highlight how solvation effects stabilize C-C coupling reactions through hydrogen bonding; demonstrate that larger cations can coordinate with the *CO+*CO moiety, disrupting hydrogen bond and inhibiting undesirable hydrogenation pathways toward C₁ products.
 - Decipher the importance of *H regulatory strategy to enhance NO₃RR: show that cation coordination impedes the water-adsorbate hydrogen bond, while *H can react with oxygen-containing species; screen single atom alloys for enhanced water dissociation as promising NO₃RR electrocatalysts.Explore complex reaction network through a graph based theoretical approach
 - Develop an automated graph-theory-based tool for constructing reaction networks and enumerating adsorption configurations.

- Analyze 1,400 possible intermediates and 2,490 potential C-N coupling modes on the Cu-N₄-C catalyst for the co-reduction of CO₂ and NO₃⁻ to urea.
- Identified key indicators, such as hydrogenation and coupling energies, for rapid screening of potential electrocatalysts.

♦ **Department of Chemical and Nano Engineering, University of California, San Diego**

Research Intern with Prof. Wanlu Li

Apr 2024 – Present (remote)

Evaluate cation-dependent hydrophobic hydration in the electric double layer

- Calculate the cavity formation energy of water molecules from AIMD trajectories, and relate it to the cation-regulated hydrogen bond network.
- Examine how the above factors can modulate the energy profiles of electrochemical processes, ultimately affecting the reaction rates or selectivity.

♦ **College of Chemistry and Chemical Engineering, Xiamen University**

Undergraduate Researcher with Prof. Jun Cheng

Jun 2020 – Jun 2022

Code development of automated workflows for efficient chemical modeling

- Design an automated workflow for convenient construction of solid-liquid interface models based on Airflow platform in Python.
- Implement local data processing, remote HPC execution submission, and concurrent task scheduling, along with interfaces for software such as LAMMPS and CP2K.
- Part of this project was later integrated into the ai2-kit package and has been utilized in several subsequent projects (<https://github.com/chenggroup/ai2-kit>).

ACADEMIC ACTIVITIES

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

Jun 2024

HONORS AND AWARDS

National Scholarship, Peking University 2024

Pacemaker to Merit Student, Peking University 2024

Second Class Scholarship, Xiamen University 2021

Academic Excellence Award, Xiamen University 2020

First Prize, China Undergraduate Mathematical Contest in Modeling 2020

First Class Scholarship, Xiamen University 2019

SKILLS

Software: VASP, CP2K, LAMMPS, ASE

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

Language Proficiency: Chinese (Native), English (Fluent, TOEFL: 103)