# 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

- **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 atomic mechanism related to electrochemical $CO_2$RR selectivity: larger cations can coordinate with the *CO+*CO moiety, and prevent the further hydrogenation of *CO toward the $C_1$ product pathway
  - Decipher the importance of *H regulatory strategy to enhance $NO_3$RR: Cation coordination impedes the hydrogen bond network, but *H can react with oxygen-containing species unaffected by cations.

  Explore complex reaction network based on a graph based theoretical approach
  - Analyze 1,400 possible intermediates and 2,490 potential C-N coupling modes on the Cu-$N_4$-C catalyst for the co-reduction of $CO_2$ and $NO_3^-$ to $C_1N_2$ products.
  - Find the hydrogenation energy of *$NH_2$ and $CO_2$, as well as their coupling energy, can serve as key indicators for the 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.

- **College of Chemistry and Chemical Engineering, Xiamen University**
  *Undergraduate Researcher with Prof. Jun Cheng* Jun 2021 – Jun 2022
  Code development of automated workflows for efficient chemical modeling
  - Design an automated workflow that facilitates the rapid 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.

## ACADEMIC ACTIVITIES

Poster Presentation, **the 34$^{th}$ Chinese Chemical Society Congress**, Guangzhou, China Jun 2024

## HONORS AND AWARDS

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