Jingdan Chen

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EDUCATION

University of Illinois at Urbana-Champaign — **Urbana, IL, USA**
Graduate Student - Department of Chemistry - *GPA: 3.9/4.0* — September 2024 – Present

Wuhan University — **Wuhan, Hubei, China**
Bachelor of Science – Chemistry - *GPA: 3.9/4.0* (Top 1) — September 2020 – June 2024

RESEARCH EXPERIENCE

Nicholas Jackson's Group — **Urbana, IL, USA**
Research Assistant, AI for Polymer Synthesis and Design — November 2024 - Present

- **DFT Calculation and ML Pipeline for Polymer Reactivity:** Combining state-of-the-art machine learning model with DFT calculation to address reactivity problems in polymerization process.
- **Scientific Dataset Construction:** Extracting data from unstructured scientific text using natural language processing, including LLM, and cheminformatics tools.

Christopher Rowley's Group — **Ottawa, ON, Canada**
Summer Research Internship, Alchemical Molecular Dynamics — July 2023 – October 2023

- **Molecular Dynamics Simulation:** Determine absolute protein-ligand binding free energy change with Free Energy Perturbation theory with neural network potential aided molecular dynamics.

Xiaotian Qi's Group — **Wuhan, Hubei, China**
Undergraduate Researcher, DFT for Organic Catalysis — September 2022 – June 2024

- **DFT Calculation:** Carried out the theoretical studies to chiral phosphoric acid(CPA) catalyzed asymmetric decarboxylative protonation, clarified mechanisms and the origin of enantioselectivity.
- **Chemistry LLM:** Collaboration project, with the role of conducting cheminformatics investigation, including the fine-tunning of large language model for chemistry purpose.

Yanyan Zhang's Group — **Hangzhou, Zhejiang, China**
Summer Research Internship, DFT for PFASs Degradation — July 2022 – September 2022

- **Mechanistic Study**: Using HPLC-MS and DFT calculation to investigate the spontaneous defluorination mechanism of various PFASs.

PUBLICATIONS

1. **J. Chen**, N.E. Jackson*. A Machine Learning Model for Copolymer Radical Reactivity Ratio Predictions with Frontier-Orbital Insights. *Chem. Mater.* **37***, 7894–7907* (2025)
2. Z. Guo, G. Tremblay, **J. Chen**, S. Joudan*. Spontaneous Aqueous Defluorination of Trifluoromethylphenols: Substituent Effects and Revisiting the Mechanism. *Environ. Sci.: Process. Impacts*., **27**,1852 (2025)
3. D. Zhang‡, W. Liu‡, T. Qian‡, **J. Chen**‡, Y. Li* *et al*. Chemllm: A chemical large language model. *arXiv:2402.06852* (2024).
4. Z. Chen, **J. Chen,** Y. Zhang*, *et al*. Dechlorination helps defluorination: Insights into the defluorination of florfenicol and DFT calculations on the reaction pathways. *Environ. Sci. Technol.*, **5**, 2542–2553 (2024)

5. W. Zheng, **J. Chen**, X. Qi*, Z. Huang*. Asymmetric decarboxylative protonation enabled by an anchoring group that enhances noncovalent interactions. *Nat. Chem.,* **15**, 1672–1682 (2023)

TEACHING EXPERIENCE

University of Illinois at Urbana-Champaign **Urbana, IL, USA**

Teaching Assistant, Data Science for Chemistry and Engineering (Chem 452). Sept. 2025 – Dec. 2025

Teaching Assistant, Elementary Organic Chemistry (Chem 232) Sept. 2024 – May 2025

Wuhan University **Wuhan, Hubei, China**

Teaching Assistant, General Chemistry Sept. 2021 – May 2022

CONFERENCE PRESENTATION

1. **J. Chen**, N.E. Jackson. A Machine Learning Model for Copolymer Radical Reactivity Ratio Predictions with Frontier-Orbital Insights. ACS Spring Meeting, Atlanta, GA, USA, 2026 (Oral)
2. **J. Chen**, X. Qi. Quantitative Steric-Electronic Effect Dissection (QSED) Model for Asymmetric Protonation. The 34th CCS Congress, Guangzhou, China, 2024 (Poster)
3. **J. Chen**, X. Qi. DFT Oriented Mechanism Investigation on Asymmetric Decarboxylative Protonation of Aminomalonic Acids. The 23rd International Conference on Organic Synthesis, Shanghai, China, 2023 (Oral)