

Jingdan Chen

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GPA: 3.90/4.00 (Core-GPA: 3.97/4.00)

EDUCATION

- Wuhan University, Wuhan, China (Undergraduate Student) **09/2020 – present**
- Carleton University, Ottawa, Canada (Visiting Student) **07/2023 – 10/2023**
- Westlake University, Hangzhou, China (Visiting Student) **06/2022 – 08/2022**

PUBLICATIONS

1. Wei-Feng Zheng, **Jingdan Chen**, Xiaotian Qi*, Zhongxing Huang*. Asymmetric decarboxylative protonation enabled by an anchoring group that enhances noncovalent interactions. (*Nat. Chem.*, **15**, 1672–1682 (2023), DOI: 10.1038/s41557-023-01362-3)
2. Zhenhuan Chen, **Jingdan Chen**, Yanyan Zhang*, Shendong Tan, Zilin Yang. Dechlorination helps defluorination: Insights into the defluorination of florfenicol and DFT calculations on the reaction pathways. (*Environ. Sci. Technol.*, **5**, 2542–2553 (2024), DOI: 10.1021/acs.est.3c07435)

RESEARCH EXPERIENCE

Summer Research (Assistant professor Christopher Rowley as supervisor) **07/2023 – 10/2023**

Alchemical Simulation for Protein-Ligand Binding Free Energy Calculation

- *Rowley's Group Website*: Rowley Group
- ✧ Determine absolute protein-ligand binding free energy change with Free Energy Perturbation theory which is implemented with existing open neural network potential aided molecular dynamics.

Undergraduate Researcher (Professor Xiaotian Qi as supervisor) **09/2021 – 07/2023**

DFT-Oriented Homolysis Catalysis Mechanism Investigation

- ✧ Carried out the theoretical studies to chiral phosphoric acid(CPA) catalyzed asymmetric decarboxylative protonation, clarified mechanisms with DFT calculation and the origin of enantioselectivity with IGMH and ALMO-EDA. (See **Publication 1**)
- ✧ DFT-oriented cobalt complex catalytic mechanism and the nature of cobalt-radical interaction

investigation, mainly concentrating on “Cobalt Catalyzed contra-Thermodynamic Positional Alkene Isomerization”.

- ✧ Cheminformatics investigation, including the usage of language model in chemistry domain (Cooperated with Dr. Mao Su)

Summer Research(Assistant professor Yanyan Zhang as supervisor)

06/2022 – 08/2022

Theoretical Investigation into Per-/Poly-fluoroalkyl Substances (PFASs) Degradation

- *Zhang’s Group Website:* Alumni-environ-chem lab (westlake.edu.cn)
- ✧ Preliminarily developed the computational chemistry workflow and configured High-Performance Computing environment for Zhang’s lab.
- ✧ Conducted DFT calculation with Gaussian 16 to investigate the spontaneous defluorination mechanism of various PFASs. (see **Publication 2**)

INVITED TALKS

Oral Report at The XXIII International Conference on Organic Synthesis (23-ICOS)

19/10/2023

DFT oriented mechanism investigation on asymmetric decarboxylative protonation of aminomalonic acids

TEACHING EXPERIENCE

Teaching Assistant (Inorganic Chemistry, Professor Gongzhen Cheng’s Class)

09/2021 – 01/2022

- ✧ Assisted in preparing coursework and helped with professional knowledge and coursework for students.

SELECTED HONORS AND AWARDS

- ✧ China National Scholarship (**National Highest Scholarship**, continue for two years) **12/2021&2022**
- ✧ Merit Student with First-Class Scholarship, Wuhan University (continue for two years) **10/2021&2022**
- ✧ Bronze Award of the 7th China International College Students’ ‘Internet+’ Innovation and Entrepreneurship Competition, Hubei Province **07/2021**
- ✧ National Second Prize of the 12th Lan Qiao Cup Collegiate Programming Contest, Python **06/2021**