

シュウ ダイチ
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EDUCATION

Fudan University 复旦大学 September 2019 – June 2023
Bachelor of Science in Chemistry, Minor in Software Product Designing Shanghai, China

- **GPA** Senior year 3.1/4.0, Minor Courses 3.55/4.0
- **Relevant Coursework:** Organic Chemistry (A), Computational Chemistry (A-), Python Programming (A), Software Engineering (A), Software Technology of Industrial Internet (A-), Database Design, System Programming
- **Thesis Title:** Density Functional Theory (DFT) Computational Study on the Selective Borylation of Adenosine C-H Bonds
- **Thesis Advisor:** Prof. Zhiming Li
- **Award:** 2021-2022 Fudan University Undergraduate Professional Scholarships

The University of Tokyo 東京大学 October 2024 – Present
Master Student in Computational Biological Science Program, GSFS Kashiwa, Chiba, Japan

- **Supervisor:** Prof. Koji Tsuda
- **Lab Website:** [🔗 Tsuda Lab](#)
- **Research Interest:** AI4S, Computational Drug Discovery, Graph Neural Networks

RESEARCH

DFT Computational Study on Regioselective Homolytic C²-H Borylation of Unprotected Adenosine and Adenine Derivatives via Minisci Reaction January 2023 – January 2024

Supervisor: Prof. Zhiming Li, Dept. of Chemistry, Fudan University Shanghai, China

- Applied DFT to computationally validate boramine radicals' reactivity, which could provide a theoretical foundation for synthesizing bioactive molecules and drug development.
- Explained the promotional effect of adding MgCl₂ in the reaction by calculating the free energy barrier of the reaction, and conducted NPA charge analysis on reactant fragments along with IGMH analysis on transition state structures to further understand this reaction.
- **Publication:** Li, Y.; Zhou, Y.; Zhou, D.; Jiang, Y.; Butt, M.; Yang, H.; Que, Y.; Li, Z.; Chen, G. *Regioselective Homolytic C²-H Borylation of Unprotected Adenosine and Adenine Derivatives via Minisci Reaction*, *J. Am. Chem. Soc.* **2024**, *146* (31), 21428–21441. DOI: [🔗 10.1021/jacs.4c03865](https://doi.org/10.1021/jacs.4c03865)
- **Collaboration (Wet Lab):** Prof. Gang Chen's group, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, Shanghai, China

EMPLOYMENT

Software Development and Machine Learning Engineer (Remote) September 2023 – March 2024

QuanMol Tech, Inc. [🔗 Website](#) San Carlos, CA, United States

- Contributed to the development of QuanMol *ReDefine* [🔗](#), an advanced, data-secure, AI-driven *in-silico* platform.
- Trained LSTM & CNN models on organic molecule structures and their SMILES identifiers.
- Managed database administration & backend framework with MySQL, Redis, and Kubernetes, and optimized the interface for protein and drug molecule localization and compatibility scoring.

ADDITIONAL INFORMATION

- **Programming Skills:** Python, C, Shell, Java, PyTorch, TypeScript
- **Softwares:** Git, Docker, Kubernetes, MySQL, Redis, \LaTeX , MATLAB, ChemDraw, Gaussian
- **Languages Proficiency:** Chinese (Native), English (Fluent), Japanese (Daily Conversation)
- **Certifications:** TOEFL 105 (Reading 29, Listening 28, Speaking 21, Writing 27), GRE 322 (Verbal 152, Quantitative 170), Academic Writing 4.0