ZHOU, Dazhi 周大智 (シュウ ダイチ)

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Education

The University of Tokyo 東京大学 Oct. 2026 – Present
Doctoral Course, Department of Computational Biology and Medical Sciences Kashiwa, Chiba, Japan

- **Graduate School**: Frontier Sciences **Advisor**: Prof. Koji Tsuda Tsuda Lab
- **Research Focus**: AI for Chemistry, Density Functional Theory (DFT), Machine Learning, Transition State Search

The University of Tokyo 東京大学 Oct. 2024 – Sept. 2026
Master of Science, Department of Computational Biology and Medical Sciences Kashiwa, Chiba, Japan

- **Graduate School**: Frontier Sciences **Advisor**: Prof. Koji Tsuda

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

- **Thesis**: Density Functional Theory (DFT) Computational Study on the Selective Borylation of Adenosine C–H Bonds (Advisor: Prof. Zhiming Li)
- **Relevant Coursework**: Organic Chemistry (**A**), Computational Chemistry (**A-**), Python Programming (**A**), Software Engineering (**A**), Software Technology of Industrial Internet (**A-**), Database Design, System Programming
- **Award**: Fudan University Undergraduate Professional Scholarship, 2021–2022

Fellowships & Awards

JST SPRING GX Doctoral Fellowship Oct. 2026 – Present
The University of Tokyo · Japan Science and Technology Agency (JST)

- Competitively selected fellow of the University of Tokyo's SPRING GX (Green Transformation) program, funded by JST's *Support for Pioneering Research Initiated by the Next Generation* (SPRING).

Research Experience

Graduate Research, Tsuda Lab Oct. 2024 – Present
Supervisor: Prof. Koji Tsuda, The University of Tokyo Kashiwa, Chiba, Japan

- Data-driven molecular design combining machine learning with quantum-chemical (DFT / TD-DFT) calculations.
- **Student Trainee**, Molecular Informatics Team, RIKEN Center for Advanced Intelligence Project (AIP), Jan. 2025 – Sept. 2026.

DFT Mechanistic Study of Nucleoside Carboranylation Jan. 2025 – Apr. 2026
Supervisor: Prof. Zhiming Li, Dept. of Chemistry, Fudan University Remote, based in Japan

- Performed DFT calculations to elucidate the substrate-dependent regioselectivity of Minisci-type carboranylation at unprotected nucleosides, revealing that C2-selectivity in adenosine arises from steric repulsion while C5-selectivity in uridine is governed by stabilizing interactions.
- **Outcome**: Co-first-author article in *J. Am. Chem. Soc.* (2026) [P2].
- **Collaboration (Wet Lab)**: Prof. Gang Chen's group, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University

DFT Mechanistic Study of Adenosine C^2–H Borylation Jan. 2023 – Jan. 2024
Supervisor: Prof. Zhiming Li, Dept. of Chemistry, Fudan University Shanghai, China

- Applied density functional theory (DFT) to computationally validate the reactivity of boramine radicals, providing a theoretical foundation for synthesizing bioactive molecules and drug development.
- Explained the promotional effect of $MgCl_2$ on the reaction by calculating free-energy barriers, and conducted NPA charge analysis on reactant fragments and IGMH analysis on transition-state structures.
- **Outcome**: Co-first-author article in *J. Am. Chem. Soc.* (2024) [P1].
- **Collaboration (Wet Lab)**: Prof. Gang Chen's group, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University

Publications

[P2] Zhou, Y.†; Bag, R.†; Zhou, D.†; Jiang, Y.; Que, Y.; Xie, R.; Wang, R.; Li, Y.; Li, Z.; Chen, G. Late-Stage Carboranylation of Nucleos(t)ides Enabled by Minisci and Pd-Catalyzed B–N Cross-Coupling Reactions: Toward the Synthesis of Carboranyl-Modified Oligonucleotides. *J. Am. Chem. Soc.* **2026**, *148* (25), 26629–26648. DOI: 10.1021/jacs.6c07376

[P1] Li, Y.[†]; Zhou, Y.[†]; Zhou, D.[†]; Jiang, Y.; Butt, M.; Yang, H.; Que, Y.; Li, Z.; Chen, G. Regioselective Homolytic C^2–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

[†]Equal contribution.

Presentations

Data-Driven Design of Solvatochromic Fluorophores with a Small Benzene Core Mar. 2026
The 106th CSJ Annual Meeting, Nihon University, Funabashi, Chiba, Japan Poster

- **Authors**: Dazhi Zhou, Sourav Mete, Kei Terayama, Masato Sumita, Ryo Tamura, Masanobu Naito, Koji Tsuda
- **Keywords**: Solvatochromism, Fluorescence, TD-DFT, Data-Driven Molecule Design, Machine Learning

Industry Experience

Software Development and Machine Learning Intern Sept. 2023 – Mar. 2024
QuanMol Tech, Inc. Website · Remote, Part-time 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.

Skills & Languages

- **Computational Chemistry**: Gaussian, DFT / TD-DFT, NPA, IGMH, ChemDraw
- **Programming**: Python, PyTorch, C, Shell, Java, React.js, MATLAB
- **Tools**: Git, Docker, Kubernetes, MySQL, Redis, LaTeX
- **Languages**: **Chinese** (Native), **English** (Fluent), **Japanese** (Daily Conversation)
- **Test Scores**: **TOEFL** 105 (R29, L28, S21, W27); **GRE** 322 (V152, Q170, AW4.0)