Renjie Zhu

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EDUCATION

East China Normal University (ECNU), Shanghai, China 2021/08 – 2025/07

Bachelor of Science in Chemistry

- **Overall GPA**: 3.88/4.0; 92/100

Boston University, Boston, United States 2025/08 – Present

Chemistry Ph.D. program

RESEARCH EXPERIENCE

Project 1: *CG model development and theoretical simulation of microtubule* 2022/01 – 2024/12

National Innovation and Entrepreneurship Training Program for College Students

***Project Leader* (NYU-ECNU Center for Computational Chemistry)**

Supervisor: Assoc. Prof. Fei Xia

- Proposed an efficient method for coarse-grained modeling of microtubules based on helical features
- Completed theoretical simulation studies of microtubule physical properties and biological processes

Project 2: *Protein pocket alignment based on surface fingerprint* 2024/07 - 2024/08

Westlake University Summer Internship Program

Supervisor: Assoc. Prof. Jing Huang

- Proposed an alignment framework based on the surface properties of protein pockets
- Designed a similarity scoring function and completed some basic benchmarking tests

Project 3: *Optimized L-J Parameters of Martini3 Small Organic Molecules* 2024/12 – 2025/08

Supervisor: Assoc. Prof. Fei Xia

- Applied Lennard-Jones Static Potential Matching method (LJSPM) to get "bottom-up" L-J parameters of small molecules from AA force field
- Performed CGMD simulations using optimized L-J parameters for validation

PUBLICATIONS

1. **Zhu, R**., Zhu, T., Wu, R., & Xia, F. Optimized Lennard-Jones Parameters Improve Martini3 Force Fields for Small Organic Molecules. (In Preparation)
2. **Zhu, R**., Zhang, Y., Zhu, T., & Xia, F. (2025). Coarse-Grained Simulation of Persistence Length and Twisting Dynamics of Micrometer-Scale Microtubules. *The Journal of Physical Chemistry Letters*, *16*, 7300-7306.

HONORS & AWARDS

Outstanding Undergraduate Thesis of ECNU 2025/06

Outstanding Graduates in Shanghai 2025/05

National Scholarship for Undergraduate Students (For Top 1) 2024/12

18th Shanghai College Students' Chemistry Experiment Competition Special Prize (Top 1) 2024/07

Special Scholarship for Outstanding Students of ECNU 2023/12
Outstanding Report Award of the 9th ECNU Undergraduate Innovation and Entrepreneurship Academic Forum 2023/12
Outstanding Undergraduate Students of ECNU 2023/12
Contemporary Undergraduate Mathematical Contest in Modeling Second Prize (Top 3%) 2023/11
17th Shanghai College Students' Chemistry Experiment Design Competition Special Prize (Top 1) 2023/08
National Scholarship for Undergraduate Students (For Top 1) 2022/12
Outstanding Undergraduate Student Cadre of ECNU 2022/12

LANGUAGES & SKILLS

Languages: Mandarin (Native), English (IELTS: 7.5)
Computer Skills: Python, Linux, LAMMPS, GROMACS, Discovery Studio, Origin, AI&PS