

Renjie Zhu

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EDUCATION

East China Normal University (ECNU), Shanghai, China	2021/08 – 2025/07
<i>Bachelor of Science in Chemistry</i>	
➤ Overall GPA: 3.88/4.0; 92/100	
Boston University, Boston, United States	2025/08 – Present
<i>Chemistry Ph.D. program</i>	

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	
<i>Project Leader (NYU-ECNU Center for Computational Chemistry)</i>	
<i>Supervisor: Assoc. Prof. Fei Xia</i>	
➤ 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	
<i>Supervisor: Assoc. Prof. Jing Huang</i>	
➤ 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
<i>Supervisor: Assoc. Prof. Fei Xia</i>	
➤ 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. (2025). Optimized Lennard-Jones Parameters Improve Martini3 Force Fields for Small Organic Molecules. *ChemRxiv*.
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
18 th 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 9 th 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
17 th 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