

Renjie Zhu

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EDUCATION

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

RESEARCH EXPERIENCE

Project 1: <i>CG model development and theoretical simulation of microtubule</i> National Innovation and Entrepreneurship Training Program for College Students Project Leader (NYU-ECNU Center for Computational Chemistry) Supervisor: <i>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	2022/01 – 2024/12
Project 2: <i>Protein pocket alignment based on surface fingerprint</i> Westlake University Summer Internship Program Supervisor: <i>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	2024/07 - 2024/08
Project 3: <i>Optimized L-J Parameters of Martini3 Small Organic Molecules</i> Supervisor: <i>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	2024/12 – 2025/08

PUBLICATIONS

- Zhu, R.**, Zhu, T., Wu, R., & Xia, F. (2025). Optimized Lennard-Jones Parameters Improve Martini3 Force Fields for Small Organic Molecules. *ChemRxiv*.
- 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