

RENJIE ZHU

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590 Commonwealth Avenue, Boston, MA, 02215, United States

EDUCATION

Boston University
Chemistry Ph.D. program

Aug 2025 - Present
Advisor: Qiang Cui

East China Normal University (ECNU)
B.Sc. in Chemistry (Rank 1/59)

Aug 2021 - Jul 2025
Advisor: Fei Xia

RESEARCH EXPERIENCE

Department of Chemistry, Boston University
Advisor: Prof. Qiang Cui

Aug 2025 - Present
Graduate Student Researcher

- Use MD-based computational approaches to uncover allosteric behaviors in protein complexes.

School of Life Sciences, Westlake University
Supervisor: Prof. Jing Huang

Jul 2024 - Aug 2024
Summer Internship

- Propose an alignment framework based on the surface properties of protein pockets, design a similarity scoring function, and complete some basic benchmarking tests.

NYU-ECNU Center for Computational Chemistry, ECNU
Advisor: Prof. Fei Xia

Jan 2022 - Aug 2025
Undergraduate Researcher

- Propose an efficient method for CG modeling of microtubules based on helical features and complete theoretical simulation studies of physical properties and biological processes.
- Apply Lennard-Jones Static Potential Matching method (LJSPM) to get “bottom-up” L-J parameters of CG small molecules from AA force field.
- Project Leader of the National Innovation and Entrepreneurship Training Program for College Students.

SCHOLARSHIPS & AWARDS

Outstanding Undergraduate Thesis, ECNU	Jun 2025
Outstanding Graduates in Shanghai, Shanghai Municipal Education Commission	May 2025
Outstanding Undergraduate Students, ECNU	Dec 2023
Special Scholarship for Outstanding Students, ECNU	Dec 2023
Outstanding Report Award in 9 th Undergraduate Innovation and Entrepreneurship Academic Forum, ECNU	Dec 2023
Outstanding Undergraduate Student Cadre, ECNU	Dec 2022
National Scholarship for Undergraduate Students, Ministry of Education, PRC	2022, 2024

PUBLICATIONS

1. Shi, J.; Wan, Z.; **Zhu, R.**; Cui, Q.*; Measuring Differences in Protein Allosteric Graphs Constructed via Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2026**, *22*, 6180–6195.
2. **Zhu, R.**; Zhu, T.; Wu, R.; Xia F.*; A Coarse-Grained Model for Small Organic Molecules with Opti-

mized Lennard-Jones Parameters. *The Journal of Physical Chemistry B*, **2026**.

3. Zhu, R.; Zhang Y.; Zhu, T.; Xia F.*, Coarse-Grained Simulation of Persistence Length and Twisting Dynamics of Micrometer-Scale Microtubules. *The Journal of Physical Chemistry Letters*, **2025**, *16*, 7300–7306.

TEACHING

Teaching Assistant of CASCH 102: General Chemistry 2 (LAB section), Boston University Spring 2026