

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
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- 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
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- 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
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- 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. *In Submission*, **2026**.
2. **Zhu, R.**; Zhu, T.; Wu, R.; Xia F.* , Enhancing the Simulation Accuracy of Small Organic Molecules

with an Optimized Lennard-Jones Coarse-Grained Model. *preprint on ChemRxiv*, **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