Qingshi Wang

qw293@cornell.edu · (607) 279-3247 · ORCID · Github · Personal Website

SUMMARY

I am currently concentrating on polymer modeling, structural and mechanical properties. I have managed to build complex polymer models for LAMMPS simulation. In the future, I am eager to devote myself to new property discovery and material design using quantum computation, Molecular Dynamics simulation and machine learning techniques.

EDUCATION

Cornell University   Ithaca, NY
Master of Science in Materials Science and Engineering, Advisor: Jingjie Yeo   *Expected June 2026*
Thesis: Molecular Simulations on Polymer Entanglement
- Built polymer models and studied the impacts of chain entanglement on polymer properties.

East China University of Science and Technology   Shanghai, China
Bachelor of Engineering in Polymer Materials and Engineering, Advisor: Chunhua Cai   *June 2024*
Thesis: Synthesis of Polylysine and its Self-assembly Research
- Synthesized polylysine and characterized self-assemble behavior by environmental changes.

RESEARCH EXPERIENCE

Relationship of polymer entanglement and mechanical properties   Ithaca, NY
Graduate Researcher, Jingjie Yeo Group at Cornell University   *Aug 2024-Present*

- Concentrated on various polymers and polymer-based composites, and interested in mechanical properties regulated by polymer entanglements.
- Developed Python scripts to create polymer models based on Monte Carlo (MC) theories for simulation and characterized elastic constants influenced by chain constraint.
- Designed dynamics simulations to study entanglement effects during tensile, shearing and crystallization, and set variable conditions to determine factors influencing entanglements.
- Attempted data-based and machine learning strategies in mechanics and chemical reactions for new material design and new material discovery.

Intermolecular Interaction Research on water and macromolecules   Remote
Undergraduate Researcher, Erik Luijten Group at Northwestern University   *Feb 2023-Mar 2023*

- Understood significance of Molecular Dynamics simulations in biomedical engineering, organic chemistry and materials science.
- Ran LAMMPS to simulate diffusion and adsorption of water, and extended scripts to simulate expansion of PDMS in 3 solvents.
- Analyzed radical distribution function of solvent molecules and chain orientations of the systems for hydrophobic soft matter design.
- Bridged hands-on polymer synthesis experiences and computational research, comprehending accuracy, degree of approximation and effectiveness of simulations.

Preparation and Performance Study of pH-sensitive Microneedles   Shanghai, China
Undergraduate Researcher, Hongyan He Group at ECUST   *Mar 2022-Oct 2023*

- Read literature and summarized development of microneedle materials and stimulus-responsive polymers for biomedical applications.

- Synthesized 4 sorts of pH-sensitive hydrogel and selected poly acrylic acid (PAA) to manufacture microneedle arrays.
- Adjusted ratios of reactants and leveraged photocrosslinking to improve the efficiency of polymerization of PAA and developed a high-speed synthesis strategy to fabricate PAA microneedles.
- Observed microscopic geometry of microneedles using SEM and TEM, tested tensile, compression and shearing strength of the hydrogel and made cellular toxicity experiments for further applications.

WORK EXPERIENCE

Wanma Macromolecule Co., Ltd.   Zhejiang, China
Research Assistant, Department of Cable Materials   *Nov 2023-Dec 2023*

- Analyzed the formulation of PVC cable materials, shielded cable materials, and low-smoke halogen-free cable materials, conducted tests on the initial products' tensile strength, density, oxygen index, and volume resistivity.
- Grasped the operation of polymer material performance testing equipment, including universal tensile machines, oxygen index testers, constant temperature stretching boxes, kneaders, torque rheometers, etc.

BASF   Shanghai, China
Office Intern, Resin Plant   *Jul 2023-Aug 2023*

- Recorded safety inspection situations, monitored the operation status of the resin plant's control terminal system
- Acquired skills in high-altitude operations, grasped the intelligent production process of polyvinyl chloride resin and acquired partial process design skills.

CNOOC Petroleum and Refinery Research Institute Co., Ltd.   Beijing, China
Polymer Research Assistant, CNOOC Petrochemicals Research Department   *Jul 2023-Aug 2023*

- Conducted literature reviews about the properties, products, and production of polyurethane materials, grasped the difference between one and two-step production of polyurethane foam plastics, and assisted in decision-making.
- Assisted the department manager and research engineers in writing project proposals, focusing on the polymerization of polyurethane foam plastic products, and efficiently completed the tasks.

SKILL

- **Simulation:** Atomsk, Moltemplate, PACKMOL, LAMMPS, VMD, OVITO, Avogadro, Quantum ESPRESSO, VASP
- **Programming:** Python, Julia, MATLAB, HTML, CSS, Shell
- **Operating System:** Linux, Windows, MacOS

PUBLICATION

- Wang, Q. (2023). "Conventional Usages and Innovation of Microneedles." *Applied and Computational Engineering, 2023, 81-85.*   Link

PRESENTATION

- "Generation of polymer models for LAMMPS simulations with established modelers and Python." 2-minute presentation at Spring Research Symposium of Department of Mechanical and Aerospace Engineering at Cornell University, Ithaca, NY. (April 2025)

AWARDS AND HONORS

- **2023:** ECUST Undergraduate Student Scholarship
- **2022:** ECUST College Student's Innovation and Entrepreneurial Training Plan, Municipal Prize
- **2022:** ECUST Summer Holiday Volunteer Plan of the ECUST, Best Volunteer