

Qingshi Wang

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SUMMARY

I am interested in modeling polymers and comprehending the structural and mechanical properties of polymers with multiscale computational mechanics. I have managed to build synthetic polymer models for Molecular Dynamics simulation in LAMMPS and analyzed the impacts of chain entanglements on deformations. In the future, I am eager to expand my interest in both synthetic and biopolymers for property prediction and molecule design with machine learning and mechanical simulations.

EDUCATION

Cornell University

Ithaca, NY

Master of Science in Materials Science and Engineering, Advisor: Jingjie Yeo

Expected June 2026

Core Courses: Machine Learning, Molecular Simulation, Computational Mechanics, Statistical Mechanics

Thesis: Molecular Simulations on Polymer Entanglement and Mechanical Properties

- Built polymer models and studied the contribution of chain entanglement to mechanical characteristics.

East China University of Science and Technology

Shanghai, China

Bachelor of Engineering in Polymer Materials and Engineering, Advisor: Chunhua Cai

June 2024

Core Courses: Polymer Chemistry, Polymer Physics, Fluid Mechanics, Solid Mechanics, Physical Chemistry

Thesis: Synthesis of Polylysine and its Self-assembly Research

- Synthesized polylysine and characterized the self-assembly behavior due to environmental changes.

RESEARCH EXPERIENCE

Simulation of entanglements and mechanical properties of polymers

Ithaca, NY

Graduate Researcher, Jingjie Yeo Group at Cornell University

Aug 2024-Present

- Concentrated on modeling thermoplastic and thermoset synthetic polymers, and studied mechanics-structure dependence of the systems during different types of deformations and entanglement effects in the soft matters.
- Developed 2 Python repositories to create unicomponent and multicomponent polymer systems based on Monte Carlo algorithms, simplifying polymer creation and energy minimization in LAMMPS simulation.
- Visualized change in number of chain entanglements in polymers during shearing and stretching simulation, and categorized chain interpenetration of united-atom polyethylene into 4 types.
- Leveraged physics-based machine learning models to predict stress-strain relationships of united-atom polyethylene systems with adjusted number and sorts of entanglements in the system.

Simulation of diffusion and adsorption of acrylic acid molecules

Remote

Undergraduate Researcher, Erik Luijten Group at Northwestern University

Feb 2023-Mar 2023

- Modified LAMMPS scripts to simulate resolution and diffusion of acrylic acid molecules in 10 water/ethanol solutions, finding the best ratio of water and ethanol to resolve acrylic acid.
- Simulated adsorption of acrylic acid molecules on the surface of polydimethylsiloxane (PDMS) molds with 10 different degrees of polymerization.
- Helped find a promising organic solution system for the polymerization of PAA, greatly reducing time of processes of photocrosslinking.
- Assisted in selecting a PDMS mold with designed crosslinking density, manufacturing microneedle arrays with nearly perfect surface geometry.

Synthesis and Performance Study of pH-sensitive Microneedles

Shanghai, China

Undergraduate Researcher, Hongyan He Group at ECUST

Mar 2022-Oct 2023

- Analyzed literatures and summarized development of microneedle materials and stimulus-responsive polymers, and proposed 3 potential strategies to fabricate pH-sensitive hydrogels.

- Synthesized pH-sensitive hydrogels using 4 different monomers, compared pH-sensitivity of the materials, and selected PAA to manufacture pH-sensitive microneedles.
- Adjusted concentration of acrylic acid solutions, intensity and distance of light to improve the efficiency of polymerization of PAA, finding the best condition to polymerize PAA.
- Observed microscopic geometry of microneedles using SEM and TEM, tested tensile, compression and shearing strength of the hydrogel, and made cellular toxicity experiments for medical practices.

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, and characterized yield strength, oxygen index, and volume resistivity of initial products.
- 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, and participated in meetings with downstream companies.
- 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 differences between one-step and two-step production of polyurethane foam plastics.
- 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
- **Programming:** Python, Julia, MATLAB, HTML, CSS, Shell
- **Operating System:** Linux, Windows

PUBLICATION

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

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