JIALE SHI

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EDUCATION & RESEARCH EXPERIENCE

4/2022-current **Massachusetts Institute of Technology (MIT)**, Boston, MA
Postdoctoral Associate
Advisor: **Bradley Olsen, Debra Audus (NIST)**
Research: build chemical intuitive polymer similarity functions and develop complex polymer embedding algorithms for the large-scale polymer database platform digitial ecosystem and accelerate the innovation of next-generation of sustainable and functional polymeric materials via integrating machine learning, statistics, data science, chemical informatics and polymer science.

11/2017-3/2022 **University of Notre Dame**, Notre Dame, IN
Ph.D. in Chemical Engineering, GPA 4.0/4.0
Advisor: **Jonathan Whitmer**
PhD Thesis: Computing Free Energy Landscapes for Materials Design
Minor in Computational Science and Engineering
Research: calculating the free energy landscapes to explore the property mechanisms of materials and facilitating inverse design of novel materials via integrating machine learning, molecular simulation and advanced sampling in the areas of polymer-surface adhesion, liquid crystal elastic response and metal cluster isomerization.

9/2013-7/2017 **Peking University**, Beijing, China
B.S. in Chemistry, GPA 3.7/4.0 (Top 10%)

AWARDS & HONORS

2023 Future Faculty Scholar, ACS Polymeric Materials Science and Engineering (PMSE) 2023
2023 Finalist, NIST Postdoctoral & Early-career Association of Researchers (PEAR) Accolades Outstanding Technical
2023 Big Data Award at Big Data in Polymer Chemistry Session, ACS POLY 2023
2023 Selected Attendees of ACS Postdoc to Faculty (P2F) Workshop 2023
2023 Selected Attendees of Soft Matter Future Faculty Workshop 2023
2023 Winner, MIT ChemE Teach-Off 2023 Competition

2023 Travel Grant of Forum for Early Career Scientists (FECS), APS March 2023
2020 Graduate School Professional Development Grant, University of Notre Dame
2020 Graduate Student Union Conference Presentation Grant, University of Notre Dame
2020 Travel Grant of Division of Soft Matter (DSOFT), APS March 2020
2020 Outstanding Paper Award, Department of Chemical and Biomolecular Engineering, University of Notre Dame
2019 Graduate School Professional Development Grant, University of Notre Dame
2019 Graduate Student Union Conference Presentation Grant, University of Notre Dame
2019 Best Poster Award, 6th Annual Notre Dame-Purdue Soft Matter & Polymers Symposium
2014-2017 Cyrus Tang Scholarship, Peking University
2014 National Endeavor Fellowship, Peking University
2012 2nd Prize in China's National Olympic Chemistry Competition

PUBLICATIONS

First/Co-First Author Publications

1 **Jiale Shi**, Debra J. Audus, Bradley D. Olsen. "MacroSimGNN: Efficient and Accurate Calculation of Macromolecule Pairwise Similarity via Graph Neural Network." *In preparation*.

2 **Jiale Shi**, Debra J. Audus, Bradley D. Olsen. "Polymer Informatics Open Benchmark." *In preparation*.

3 **Jiale Shi**, Dylan Walsh, Nathan J. Rebello, Weizhong Zou, Michael E. Deagen, Katharina A. Fransen, Xian Gao, Bradley D. Olsen, Debra J. Audus. "Calculating Pairwise Similarity of Polymer Ensembles via Earth Mover's Distance." ***ACS Polymers Au*** 2024, 4, 1, 66–76. DOI: 10.1021/acspolymersau.3c00029

4 **Jiale Shi**, Nathan J. Rebello, Dylan Walsh, Weizhong Zou, Michael Deagen, Bruno Salomao Leao, Debra J. Audus, Bradley D. Olsen. "Quantifying Pairwise Similarity for Complex Polymers." ***Macromolecules*** 2023, 56, 18, 7344-7357. DOI: 10.1021/acs.macromol.3c00761 (Polymer similarity function is designed for the polymer search engine of Community Resource for Innovation in Polymer Technology (CRIPT))

5 **Jiale Shi**, Fahed Albreiki, Yamil J. Colón, Samanvaya Srivastava, Jonathan K. Whitmer. "Using Transfer Learning to Leverage Prior Knowledge in the Prediction of Adhesive Free Energies between Polymers and Surfaces." ***Journal of Chemical Theory and Computation***. 2023, 19, 14, 4631-4640. DOI: 10.1021/acs.jctc.2c01314

6 **Jiale Shi**, Michael J. Quevillon, Pedro Henrique Amorim Valença, Jonathan K. Whitmer. "Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning." ***ACS Applied Materials & Interfaces*** 2022, 14, 32, 37161–37169. DOI: 10.1021/acsami.2c08891

7 **Jiale Shi**, Shanghui Huang, François Gygi, Jonathan K. Whitmer. "Free Energy Landscape and Isomerization Rates of Au_4 Clusters at Finite Temperature." ***The Journal of Physical Chemistry A*** 2022, 126, 21, 3392-3400. DOI: 10.1021/acs.jpca.2c02732

8 **Jiale Shi***, Hythem Sidky*, Jonathan K. Whitmer. "Automated determination of n-cyanobiphenyl and n-cyanobiphenyl binary mixtures elastic constants in the nematic phase from molecular simulation." ***Molecular Systems Design & Engineering*** 2020, 5, 1131-1136. DOI: 10.1039/C9ME00065H (* indicates equal contribution and co-first authorship)

9 **Jiale Shi**, Hythem Sidky, Jonathan K. Whitmer. "Novel Elastic Response in Twist-bend Nematic Models." ***Soft Matter*** 2019, 15**,** 8219-8226. (**inside front cover**) DOI: 10.1039/C9SM01395D

Additional Publications

1 Kevin Maik Jablonka,..., **Jiale Shi**,..."14 Examples of How LLMs Can Transform Materials Science and Chemistry: A Reflection on a Large Language Model Hackathon." ***Digital Discovery*** 2023, 2, 1233-1250. DOI: 10.1039/D3DD00113J

2 Qianxiang Ai, Fanwang Meng, **Jiale Shi**, Brenden Pelkie, Connor W. Coley. "Extracting Structured Data from Organic Synthesis Procedures Using a Fine-Tuned Large Language Model." ***Digital Discovery*** 2024. DOI: 10.1039/D4DD00091A

3 Nathan J. Rebello, Akash Arora, Hidenobu Mochigase, Tzyy-Shyang Lin, **Jiale Shi**, Debra J. Audus, Eric. S. Muckley, and Bradley D. Olsen. "BCDB: The Block Copolymer Phase Behavior Database." ***Journal of Chemical Information and Modeling*** 2024. DOI: 10.1021/acs.jcim.4c00242

4 Joren Van Herck,.., **Jiale Shi**,..., Jonathan Whitmer,..., Berend Smit. "Assessment of Fine-Tuned Large Language Models for Real-World Chemistry and Material Science Applications." ***ChemRxiv*** 2024. DOI: 10.26434/chemrxiv-2024-mm31v

5 Katharina A. Fransen, Julia Casey, **Jiale Shi**, Natalie D. Mamrol, Gabrielle F. Godbille-Cardona, Jiarui Lu, Alex M. Zappi, Debra J. Audus, B.D. Olsen. "Predictive Modeling for Polyester Biodegradability: Insights from Augmenting Binary Co-polyester Data with a Terpolymer Library." *In Preparation.*

GRANT WRITING EXPERIENCE

2024 Contributor, EPA Research Grant Proposal. PI: Bradley Olsen.

2023 Contributor, NSF CDS&E-MSS Program Proposal. PI: Bradley Olsen.

2023 Independent MIT ChemE Postdoc Research Grant, Finalist.

TEACHING & MENTORING EXPERIENCE

Fall/2023 Mentoring Sabrina Lu through MIT Undergraduate Research Opportunities Program (UROP)

Research: Machine Learning for Polymer Classification

Spring/2023 Kaufman Teaching Certificate Program (KTCP) Participant, MIT.
Workshop series aimed at training participants in evidence-based teaching techniques, including backward design with intended learning outcomes, effective student assessment approaches, active learning strategies, inclusive teaching methods.

Spring/2019 Teaching Assistant, Chemical Engineering Thermodynamics I, University of Notre Dame

Fall/2018 Teaching Assistant, Advanced Chemical Engineering Thermodynamics, University of Notre Dame

Spring/2018 Teaching Assistant, Chemical Engineering Thermodynamics I, University of Notre Dame

Fall/2017 Teaching Assistant, Science of Engineering Materials, University of Notre Dame

LEADERSHIP & PROFESSIONAL SERVICE

2023, 2024 Reviewer for *Macromolecules*

2023 Reviewer for ACS PRF New Directions

2/2024 Session Chair, 2024 MaRDA Virtual Annual Meeting

11/2023 MESD Poster Judge, 2023 AIChE Annual Meeting

8/2023 PMSE Poster Judge, ACS Fall 2023

6/2023 Volunteer, ChemE Pride Picnic, MIT

3/2023 Session Chair, APS March Meeting 2023

9/2022-8/2023 MIT ChemE DEI Committee Postdoc Representative

9/2022-8/2023 MIT ChemE Postdoc Advisory Board Leads,

2018-2021 Graduate Student Participant, Midwest Integrated Center for Computational Materials (MICCoM)

9/2018-5/2019 Graduate Student Representative at Notre Dame Graduate Student Union (GSU), University of Notre Dame

9/2017-4/2019 Social Chair at Chemical and Biomolecular Engineering Graduate Student Organization (CBEGSO), University of Notre Dame

PRESENTATIONS

Oral Presentations

1 2023 AIChE Annual Meeting, Orlando, FL, Optimal Design of Soft Matter Via Simulation, Machine Learning and Large Language Models, Meeting the Faculty Candidate Poster Session, November 2023.

2 2023 AIChE Annual Meeting, Orlando, FL, Calculating Pairwise Similarity of Polymer Ensembles Via Earth Mover's Distance, Faculty Candidates in CoMSEF/Area 1a, November 2023.

3 2023 AIChE Annual Meeting, Orlando, FL, A Graph Neural Network Approach for Efficient and Accurate Macromolecular Similarity Calculation, November 2023.

4 ACS Fall 2023, San Francisco, CA, Earth Mover's Distance as a Metric for Calculating Pairwise Similarity of Polymer Ensembles, August 2023. **(Invited Talk)**

5 ACS Fall 2023, San Francisco, CA, Quantifying Pairwise Similarity of Complex Polymers, August 2023. (**Big Data Award**)

6 APS March Meeting 2023, Las Vegas, NV, Qualifying Pairwise Chemical Similarity of Polymers. March 2023.

7 33rd International Union of Pure and Applied Physics (IUPAP) Conference on Computational Physics (Online), Free-Energy Landscape and Isomerization Rates of Au4 Clusters at Finite Temperatures, August 2022.

8 APS March Meeting 2022, Chicago, IL, Using Transfer Learning to Leverage Prior Knowledge in the Prediction of Adhesive Free Energies between Polymers and Surfaces, March 2022.

9 2021 AIChE Annual Meeting, Boston, MA, Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning, November 2021.

10 MIT-NIST Joint-Postdoc Application Interview, Predicting Adhesive Free Energies of Polymer-Surface Interactions via Machine Learning and Transfer Learning, September 2021.

11 Virtual Polymer Physics Symposium 2021 sponsored by American Physical Society, Division of Polymer Physics, Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning, August 2021.

12 Geometry and Topology meet Data Analysis and Machine Learning (GTDAML 2021), Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning, July 2021.

13 IDEA SLAM, Soft Matter Far from Equilibrium – CHESS 2030 Workshop, Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning, June 2021.
14 ACS Spring Meeting 2021 (Online), Predicting Adhesive Free Energies of Polymer-Surface Interactions with Machine Learning, April 2021.
15 APS March Meeting 2021(Online), Free energy landscapes and transition rates of dynamic properties of Au4 neutral and charged clusters at finite temperature, March 2021.
16 Department Seminar 2020 Fall, Department of Chemical and Biomolecular Engineering, University of Notre Dame, Novel elastic response in twist-bend nematic models, October 2020. (**Invited Talk).**
17 APS March Meeting 2020, Denver, CO (moved to Online), Phase behavior and elastic response of liquid crystal mixtures in atomistic models, March 2020.
18 17th International Conference on Ferroelectric Liquid Crystals, Boulder, CO, Novel Elastic Response in Twist-bend Nematic Models, August 2019.
19 2019 Midwest Thermodynamics and Statistical Mechanics Conference (MTSM), Urbana, IL, Novel Elastic Response in Twist-bend Nematic Models, June 2019.
20 APS March Meeting 2019, Boston, MA, Twist-bend-like phases and elastic response of model bent-core liquid crystals, March 2019.
21 Computational Molecular Science and Engineering Laboratory (CoMSEL) supergroup meeting, Notre Dame, IN, Twist-bend-like phases and elastic response of model bent-core liquid crystals, February 2019.

Poster Presentations

1 20204 Polymer Physics Gordon Research Conference, Calculating Pairwise Similarity of Polymer Ensembles via Earth Mover's Distance, July 2024.
1 2024 MIT Polymer Day, Accelerating Polymer Informatics via Polymer Pairwise Similarity, May 2024.
2 2024 MaRDA Virtual Annual Meeting, Calculating Pairwise Similarity of Polymer Ensembles via Earth Mover's Distance, February 2024.
3 APS March Meeting 2023, Las Vegas, NV, Pairwise Similarity of Polymer Ensembles. March 2023.
4 6th Annual Notre Dame-Purdue Soft Matter & Polymers Symposium, West Lafayette, IN, Novel Elastic Response in Twist-bend Nematic Models, September 2019. **(Best Poster Award.)**
5 5th Annual Chemical & Biomolecular Engineering Graduate Research Symposium, Notre Dame, IN, Novel Elastic Response in Twist-bend Nematic Models, September 2019.

6 51st Midwest Theoretical Chemistry Conference (MWTCC), Notre Dame, IN, Novel Elastic Response in Twist-bend Nematic Models, June 2019.

7 6th Annual Notre Dame-Purdue Soft Matter & Polymers Symposium, West Lafayette, IN, Phase Behavior and Elasticity of Polar Liquid Crystals, September 2018.

8 4th Annual Chemical & Biomolecular Engineering Graduate Research Symposium, Notre Dame, IN, Phase Behavior and Elasticity of Polar Liquid Crystals, September 2018.