Wenlin Zhang

Dartmouth College

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Education

B.S. in Chemical Engineering, University of Minnesota, 2009-2012

Ph.D. in Chemical Engineering, Pennsylvania State University (advisors: Scott Milner and Enrique Gomez), 2012-2017

Appointments

07/2020–present Assistant Professor of Chemistry, Dartmouth College

08/2017–07/2020 Post-doctoral Research Fellow, University of Michigan (advisor: Ronald

Larson)

Honors and Awards

NSF CAREER Award, 2024

Petroleum Research Fund Doctoral New Investigator Award, American Chemical Society, 2021

Walter and Constance Burke Research Initiation Award, Dartmouth College, 2020

Finalist, Frank J. Padden Jr. Award, American Physical Society, 2017

Finalist, Excellence in Graduate Polymer Research, American Institute of Chemical Engineers, 2015

Student Awards

Graduate students

Lingyi Zou, Frank J. Padden Jr. Award Finalist, American Physical Society, 2025

Undergraduate students

Elaine Jiao, Outstanding Undergraduate Research in Computational Science (Honorable Mention), Neukom Institute, 2024

Caleb Liu, Outstanding Undergraduate Research in Computational Science (2nd Prize), Neukom Institute, 2024

Caleb Liu, Barry Goldwater scholar, 2024

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Publications (Google scholar)

At Dartmouth (undergraduate student(s) highlighted in bold)

14. "Conformation-orientation coupling governs helical polymer crystallization", Zhang, W.*, in preparation, 2024.

- 13. "Mechanically Reconfigurable Polyrotaxane Networks", Zheng, D.; Yu, Z.; Smith, C.D.; Liu, J.; Tsai, E.; Zhang, W.*; Ling, S.*; Ke, C.*, in preparation, 2024.
- 12. "Roles of interfaces in crystallization in free-standing and multi-layer polymer films", Zou, L.; Zhang, W.*, *submitted*, 2024.
- 11. "Effects of block copolymer compatibilizers and interfacial entanglements on strengthening immiscible glassy polymer blends", Zhang, Y.; Zhang, W.*, *submitted*, 2024.
- 10. "All-atom molecular dynamics simulations reveal the effects of nanoplastics on lipid membranes and vice versa", Duraes, D.S.; **Jiao**, E.L.; Zhang, W.*, *submitted*, 2024.
- 9. "Predicting molecular structure of end-functionalized pseudo-polyrotaxane using multi-scale simulations", Smith, C.D.; Ke, C.*; Zhang, W.*, Soft Matter, 2024, 20, 9068–9082.
- 8. "Interfaces and soft confinement promote crystallization in polymer nanodroplets", **Liu, C.**; Duraes, D.S.; **Jiao, E.L.**; Zhang, W.*, *MRS Adv.*, 2024.
- 7. "Effects of entanglement on polymer crystal growth and inter-crystalline phase formation", Zou, L.; Zhang, W.*, *Macromolecules*, 2024, 57, 4410–4420.
- 6. "Direct measurement of polymer chain-end-to-end distances by using RAFT chain transfer agent as the FRET acceptor", Wang, Y.; Fortenberry, A.W.; Zhang, W.; Simon, Y.C.; Qiang, Z, J. Phys. Chem. B, 2023, 127, 3100–3108.
- 5. "Mismatch in nematic interactions leads to composition-dependent crystal nucleation in polymer blends", Zhang, W.*; Zou, L., *Macromolecules*, 2023, *56*, 2234–2245.
- 4. "Nematic layers as precursors to secondary nucleation of alkane oligomer crystals revealed by molecular dynamic simulations", Gong, Y.; Zhang, W.; Larson, R.G., *Macromolecules*, 2022, 55, 6311–6320.
- 3. "Molecular dynamic simulations of the effects of entanglement on polymer crystal nucleation", Zou, L.; Zhang, W.*, *Macromolecules*, 2022, 55, 4899–4906.
- 2. "An ultra-dynamic anion cluster-based organic framework", Samanta, J.; Dorn, R.W.; Zhang, W.*; Jiang, X.; Zhang, M.; Staples, R.; Rossini, A.J.*; Ke, C.*, Chem, 2022, 1, 7–9.
- 1. "Molecular dynamics simulations of crystal nucleation near interfaces in incompatible polymer blends", Zhang, W.*; Zou, L., *Polymers*, 2021, *13*, 347.

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Prior to Dartmouth

- 16. "Inelastic neutron scattering probes intermolecular lattice modes that limit charge transport in organic semiconductors", Adhikari, J.M.; Zhan, P.; Calitree, B.D.; Zhang, W.; Fair, R.; Harrelson, T.F.; Faller, R.; Moule, A.J.; Milner, S.T.; Maranas, J.K.; Hickner, M.A.; Gomez, E.D., *submitted*, 2023.
- 15. "Effect of flow-induced nematic order on polyethylene crystal nucleation", Zhang, W.; Larson, R.G., *Macromolecules*, 2020, 53, 7650-7657.
- 14. "Modeling inter-colloidal interactions induced by adsorption of mobile telechelic polymers onto particle surfaces", Zhang, W.; Travitz, A.; Larson, R.G., *Macromolecules*, 2019, 52, 5357–5365.
- 13. "A metastable nematic precursor accelerates polyethylene oligomer crystallization as determined by atomistic simulations and self-consistent field theory", Zhang, W.; Larson, R.G., *The Journal of Chemical Physics*, 2019, 150, 244903.
- 12. "Thermal fluctuations lead to cumulative disorder and enhance charge transport in conjugated polymers", Zhang, W.; Bombile, J.H.; Weisen, A.R.; Xie, R.; Colby, R.H.; Janik, M.J.; Milner, S.T.; Gomez, E.D., *Macromolecular Rapid Communications*, 2019, 40, 1900134.
- 11. "Tension-induced nematic phase separation in bidisperse homopolymer melts", Zhang, W.; Larson, R.G., ACS Central Science, 2018, 4, 1545-1550.
- 10. "Side chain length affects backbone dynamics in poly(3-alkylthiophene)s", Zhan, P.; Zhang, W.; Jacobsm I.E.; Nisson, D.M.; Xie, R.; Weissen A.R.; Colby, R.H.; Moulé, A.J.; Milner, S.T.; Maranas, J.K.; Gomez, E.D., *Journal of Polymer Science Part B*, 2018, 56, 1193-1202.
- 9. "Direct all-atom molecular dynamics simulations of the effects of short chain branching on polyethylene oligomer crystal nucleation", Zhang, W.; Larson, R.G., *Macromolecules*, 2018, 51, 4762-4769.
- 8. "Nematic order imposes molecular weight effect on charge transport in conjugated polymers", Zhang, W.; Milner, S.T.; Gomez, E.D., ACS Central Science, 2018, 4, 413-421.
- 7. "Predicting Flory-Huggins χ from simulations", Zhang, W.; Gomez, E.D.; Milner, S.T., *Physical Review Letters*, 2017, 119, 017801.
- 6. "Using surface-induced ordering to probe the isotropic-to-nematic transition for semiflexible polymers", Zhang, W.; Gomez, E.D.; Milner, S.T., *Soft Matter*, 2016, 12, 6141-6147.
- 5. "Predicting the Flory-Huggins χ parameter for polymers with stiffness mismatch from molecular dynamics simulations", Kozuch, D.J.; Zhang, W.; Milner, S.T., *Polymers*, 2016, 8, 241.
- 4. "Molecular Rectification in Conjugated Block Copolymer Photovoltaics", Grieco, C.; Aplan, M.P.; Rimshaw, A.; Lee, Y; Le, T.P.; Zhang, W.; Wang, Q.; Milner, S.T.; Gomez, E.D.; Asbury, J.A., *Journal of Physical Chemistry C*, 2016, 120, 6978-6988.
- 3. "Surface induced alignment for semiflexible polymers", Zhang, W.; Gomez, E.D.; Milner, S.T., *Macromolecules*, 2016, 49, 963-971.
- 2. "Predicting nematic phases of semiflexible polymers", Zhang, W.; Gomez, E.D.; Milner, S.T., *Macromolecules*, 2015, 48, 1454-1462.

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1. "Predicting chain dimensions of semiflexible polymers from dihedral potentials", Zhang, W.; Gomez, E.D.; Milner, S.T., *Macromolecules*, 2014, 47, 6453-6461.

Seminars and Conference Presentations

Invited talks

- 4. "Effects of entanglement and segmental relaxation on polymer crystallization", Zhang, W., Annual Meeting of the American Institute of Chemical Engineers, San Diego, CA, October 2024.
- 3. "Towards quantitative modeling crystallization for semicrystalline polymers", Zhang, W., University of New Hampshire, Durham, NH, March 2024.
- 2. "Effect of chain stiffness on the performance of conjugated polymers", Zhang, W.; Gomez, E.D.; Milner, S.T., Frank J. Padden Award Symposium, Annual Meeting of the American Physical Society, New Orleans, LA, March 2017.
- 1. "Predicting nematic phases for semiflexible polymers from simulations", Zhang, W.; Gomez, E.D.; Milner, S.T., Excellence in Graduate Polymer Research Symposium, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT, November 2015.

Contributed presentations

- 17. Oral presentation. "Conformation-orientation coupling in helical polymers from atomistic simulations", Zhang, W., Annual Meeting of the American Physical Society, Minneapolis, MN, March 2024.
- Oral presentation. "Entanglement and amorphous segments in polymer crystal nucleation and growth", Zhang, W.; Zou, L., XIXth International Congress of Rheology, Athens, Greece, July 2023.
- 15. Oral presentation. "Atomistic simulations and theory of composition-dependent crystal nucleation in polymer blends", Zhang, W.; Zou, L., Annual Meeting of the American Physical Society, Las Vegas, NV, March 2023.
- 14. Oral presentation. "Molecular Dynamics Simulations of Composition-Dependent Crystal Nucleation in Polymer Blends", Zhang, W.; Zou, L., Annual Meeting of the American Institute of Chemical Engineers, Phoenix, AZ, November 2022.
- 13. Oral presentation. "Molecular dynamics simulations of crystal nucleation in polymer blends", Zhang, W.; Zou, L., Annual Meeting of the American Institute of Chemical Engineers, Boston, MA, November 2021.
- 12. Oral presentation. "Effects of phase separation and interfaces on incompatible polymer crystallization", Zhang, W.; Zou, L., Annual Meeting of the American Physical Society, Virtual Conference, March 2021.
- 11. Oral presentation. "Modeling Inter-Colloidal Interactions Induced by Adsorption of Mobile Telechelic Polymers onto Particle Surfaces", Zhang, W.; Larson, R.G., Annual Meeting of the American Institute of Chemical Engineers, Orlando, FL, November 2019.

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10. Oral presentation. "Tension-induced nematic phase separation in bidisperse homopolymer melt", Zhang, W.; Larson, R.G., Annual Meeting of the American Institute of Chemical Engineers, Orlando, FL, November 2019.

- 9. Poster presentation. "Role of stretched chains in flow-induced nucleation of polyethylene", Zhang, W.; Larson, R.G., Gordon Research Conferences: Crystal Growth and Assembly, Southern New Hampshire University, NH, June 2019
- 8. Oral presentation. "Tension-Induced Nematic Phase Separation in Homopolymer Melts", Zhang, W.; Larson, R.G., Annual Meeting of the American Physical Society, Boston, MA, March 2019.
- 7. Poster presentation. "Tension-induced nematic phase separation in bidisperse homopolymer melt", Zhang, W.; Larson, R.G., Gordon Research Conferences: Polymer Physics, Mount Holyoke College, MA, July 2018
- 6. Oral presentation. "Role of thermal fluctuations on local lattice disorder and charge transport in conjugated polymers", Zhang, W.; Milner, S.T.; Gomez, E.D., Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA, November 2016.
- 5. Poster presentation. "Extracting Flory-Huggins χ for polymers from simulations", Zhang, W.; Kozuch, D.J.; Gomez, E.D.; Milner, S.T., Gordon Research Conferences: Polymer Physics, Mount Holyoke College, MA, July 2016.
- 4. Oral presentation. "Surface induced alignment for semiflexible polymers", Zhang, W.; Gomez, E.D.; Milner, S.T., Annual Meeting of the American Physical Society, Baltimore, MD, March 2016.
- 3. Oral presentation. "Predicting nematic coupling constants of semiflexible polymers from MD simulations", Zhang, W.; Gomez, E.D.; Milner, S.T., Annual Meeting of the American Physical Society, San Antonio, TX, March 2015.
- 2. Poster presentation. "Extracting nematic coupling constants for semiflexible chains from simulations", Zhang, W.; Gomez, E.D.; Milner, S.T., Gordon Research Conferences: Polymer Physics, Mount Holyoke College, MA, July 2014.
- 1. Oral presentation. "Chain shapes and ordering of conjugated polymers from atomistic simulations", Zhang, W.; Gomez, E.D.; Milner, S.T., Annual Meeting of the American Physical Society, Denver, CO, March 2014.

Teaching Experience

Dartmouth College, General Chemistry II (CHEM.006), 2021 and 2022 Spring

Second part of the general chemistry sequence at Dartmouth College

Topics: Reaction Kinetics, Introductory Quantum Mechanics, Orbitals, and Bonding

Dartmouth College, General Chemistry (CHEM.011), 2022, 2023 and 2024 Fall

Accelerated general chemistry course for first-year undergraduate students with strong backgrounds in chemistry

Topics: Introductory Quantum Mechanics, Orbitals, Bonding, Thermodynamics, Electrochemistry, Reaction Kinetics

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Dartmouth College, Materials Chemistry (CHEM.261), 2021 Winter

Discussions of papers from the material chemistry literature

Dartmouth College, Introduction to Statistical Thermodynamics and molecular simulations (CHEM.101.5/96.05), 2021 Fall and 2024 Winter

A new graduate course developed for graduate and senior undergraduate students with interests in computational and theoretical research

Topics: Introduction to Statistical mechanics, Monte Carlo and Molecular dynamics simulations, mean-field theories.

Dartmouth College, Graduate Research Colloquium in Computational and Theoretical Chemistry (CHEM.265), 2023 and 2024 Winter

Discussions of papers from the theoretical and computational chemistry literature

Dartmouth College, Chemistry of Macromolecules (Chem 101.4/96.04), 2023 Spring

Introducing fundamentals of polymer science to undergraduate and graduate students at the introductory level

Topics: Polymer physics, discussion of experimental, computational, and theoretical tools for studying polymers and other macromolecules

University of Michigan, Advanced Special Topics in Chemical Engineering (ChE 496), Guest Lecturer, 2019 Winter

Topics: Introductory Statistical Mechanics, Monte Carlo Simulations

Pennsylvania State University, Process Fluid Mechanics (ChE 300), Teaching Assistant, 2015 Fall

Mentoring Experience

Dartmouth College

Post-docs

Anderson Da Silva Duraes (2023-present)

Graduate students

Lingyi Zou (2020-present), Cameron Smith (2021-present), Chengxi Li (M.S., 2022-2024,), Yunjia Zhang (2024-present)

Undergraduate students

Anna Beth Swain (2021), Ericka Asmus (2021), Sophia Ruben (2021), Carmela Ribadeneira (2022), Isadore Axinn (2022-2023), Mariana Cepeda Quintero (2023), Caleb Liu (2024-present), Elaine Jiao (2024-present)

Highschool students

Maiya Adolphus (2022, ACS Project Seed)

University of Michigan

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Graduate students

Alyssa Travitz (2017-2020), Futianyi Wang (2018-2020)

Undergraduate students

Yiheng Wu (2018)

Pennsylvania State University

Undergraduate students

Daniel Kozuch (2015-2016, with a first-author publication in *Polymers*)

Synergistic Activities

Service to Research Community

Organized and chaired the invited session "Recent Advances in Polymer Recycling, Upcycling, and Sustainability" at 2024 Annual March Meeting of the American Physical Society

Initiated and chaired focus sessions about "Physics in Polymer Recycling and Upcycling" at Annual March Meetings of the American Physical Society (2022, 2023, 2024)

Co-chaired sessions "Polymer Simulations: Methods and Applications " and "Polymer Simulations: Structure and Fundamental Insights" for Annual meeting of the American Institute of Chemical Engineers (2022)

Invited chair for session "Sustainable and Recyclable Polymers" at Annual Meeting of the Society of Rheology (2022)

Referee Service

The Journal of Physical Chemistry, The Journal of Chemical Information and Modeling, Macromolecules, Macromolecular Theory and Simulations, Polymer, Industrial & Engineering Chemistry Research, Journal of Polymer Science, Polymer Chemistry, National Science Foundation

STEM Outreach

Mentoring female undergraduate students on research through the Women in Science Project (WISP) program at Dartmouth College

Mentoring high students from underrepresented minority group through ACS Project Seed

Mentoring an African American high school student from a low-income family

Developing open source (Python and Jupyter Notebook based) research training module for enhancing remote/virtual research experience

Demonstrations of molecular dynamics simulations during the National Chemistry Week

Demonstration of Green Chemistry and Plastic recycling for Science Day at Dartmouth

Departmental Service

Dartmouth Chemistry Graduate Student Entrance Committee (GSEC) member (2020-2021) and chair (2022-present), Seminar Committee member (2020-2021), Curriculum Committeemember (2021-2022), Faculty Search Committee member (2021-2022), Safety Committee member (2022-2023)

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Professional Affiliations

Member, American Physical Society

Member, American Institute of Chemical Engineers

Member, American Chemical Society

Member, Society of Rheology