Dr. Ning Wang

Phone: 2672755594 Email Personal Email LinkedIn Google scholar ORCID

Expertise: Molecular modeling and simulation, free energy calculations, machine learning techniques, large language models, and force field development

Education

August 2020 to May 2024 **Ph.D. in Chemical Engineering, University of Notre Dame**, GPA: 4.0/4.0
Dissertation: Development of advanced computational methods for accurate property prediction of fluids: Application to hydrofluorocarbon/ionic liquid mixtures
Advisor: Dr. Edward J. Maginn

August 2018 to May 2020 **M.S.E. in Materials Science and Engineering, University of Pennsylvania**, GPA: 3.78/4.0
Advisor: Dr. Robert Riggleman

September 2014 to June 2018 **B.E. in Polymer Materials and Engineering, Beijing University of Chemical Technology**
Thesis: Design and properties of natural polymer surgical dressing
GPA: 89.28/100 (top 5%)

Professional Experience

September 2025 to Present **Assistant Professor**
Jasper Department of Chemical Engineering
The University of Texas at Tyler, Tyler, TX, USA

June 2024 to May 2025 **Postdoctoral Research Associate**
Department of Chemical & Biomolecular Engineering
University of Illinois at Urbana-Champaign, Urbana, IL, USA

Summer 2023 **Computational Modeling Intern**, Corteva Agriscience, Indianapolis, IN, USA

Publication

Ning Wang, Development of advanced computational methods for accurate property prediction of fluids: Application to hydrofluorocarbon/ionic liquid mixtures, University of Notre Dame, 2024

Kalin Baca, Karim Al-Barghouti, **Ning Wang**, et al., "Ionic liquids for the separation of fluorocarbon refrigerant Mixtures", *Chem. Rev.*, 2024, 124, 9, 5167–5226

Ning Wang and Edward J. Maginn*, "GAFF-based polarizable force field development and validation for ionic liquids", *J. Phys. Chem. B*, 2024, 128, 3, 871-881(GitHub)

Ning Wang, Montana N. Carlozo, Eliseo Marin-Rimoldi, Bridgette J. Befort, Alexander W. Dowling, Edward J. Maginn*, "Machine learning-enabled development of accurate force fields for refrigerants", *J. Chem. Theory Comput.*, 2023, 19, 14, 4546–4558 (GitHub)

Ning Wang, Ryan S. DeFever, Edward J. Maginn*, "Alchemical free energy and Hamiltonian replica exchange molecular dynamics to compute hydrofluorocarbon isotherms in imidazolium-based ionic liquids", *J. Chem. Theory Comput.*, 2023, 19, 11, 3324–3335 (GitHub) *CBE Outstanding Paper

Ning Wang, Yong Zhang, Karim S. Al-Barghouti, Rajkumar Kore, Aaron M. Scurto, Edward J. Maginn*, "Structure and dynamics of hydrofluorocarbon/ionic liquid mixtures: An experimental and molecular dynamics study", *J. Phys. Chem. B*, 2022, 126, 41, 8309–8321

Ning Wang, Yong Zhang, Edward J. Maginn*, "Molecular dynamics study of the ionic liquid 1-n-hexyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ($[C_6C_1im][FAP]$): Force field development and the effect of $[FAP]^-$ isomer content on properties", *J. Ionic Liq.*, 2(2022) 100040 (Journal cover)

Tianren Zhang, **Ning Wang**, Robert A. Riggleman*, "Failure and Mechanical Properties of Glassy Diblock Copolymer Thin Films", *Macromol.*, 2022, 55, 24, 10880-10890

Hongwei Zhang, Qijian Niu, **Ning Wang**, Jun Nie, Guiping Ma*, "Thermo-sensitive drug controlled release PLA core/PNIPAM shell fibers fabricated using a combination of electrospinning and UV photopolymerization", *Eur. Polym. J.*, 71(2015) 440-450

Conference

First-authored:

- Oral Presenter, "GAFF-Based Polarizable Force Field Development and Validation for Ionic Liquids", AFOSR Ionic Liquids Working Group, virtual, November 15, **2023**.
- Oral and Poster Presenter, "Machine Learning Enabled Development of Accurate Force Fields for Refrigerants", 2023 AIChE Annual Meeting, Orlando, FL, USA, November 5-10, **2023**.
- Oral Presenter, "Elucidating the effect of ionic liquid structure on the separation of hydrofluorocarbon mixtures: A molecular modeling study", 2022 AIChE Annual Meeting, Session: Thermodynamics at the Nanoscale, Phoenix, AZ, USA, November 17, **2022**.
- Oral and Poster Presenter, "Hamiltonian Replica Exchange Simulations of Hydrofluorocarbon Solubility in Ionic Liquids", Gordon Research Seminar on Chemical Separations and Gordon Research Conference on Chemical Separations, Ventura, CA, USA, October 1-7, **2022**.
- Poster Presenter, "Hamiltonian Replica Exchange Simulations of Hydrofluorocarbon Solubility in Ionic Liquids", Gordon Research Seminar on Ionic Liquids and Gordon Research Conference on Ionic Liquids, Newry, ME, USA, August 6-12, **2022**.
- Poster Presenter with FOMMS 2022 Early Career Researcher Award by the US National Science Foundation (NSF), "Hamiltonian Replica Exchange Simulations of Hydrofluorocarbon Solubility in Ionic Liquids", Foundations of Molecular Modeling and Simulation, Delavan, WI, USA, July 17-21, **2022**.
- Oral Presenter, "Elucidating the effect of ionic liquid structure on the separation of hydrofluorocarbon mixtures: A molecular modeling study", ACS 26^{th} Annual Green Chemistry and Engineering Conference - Refrigerant Symposium, Reston, VA, USA, June 6, **2022**.
- Oral Presenter, "Elucidating the effect of ionic liquid structure on the separation of hydrofluorocarbon mixtures: A molecular modeling study", Midwest Thermodynamics and Statistical Mechanics Conference, University of Wisconsin-Madison (virtual), WI, USA, June 16, **2021**.

Co-authored:

- Montana Carlozo, **Ning Wang**, Alexander Dowling, Edward Maginn, "Systematically Building and Optimizing a Generalized Hydrofluorocarbon Refrigerant Force Field", 2025 AIChE Annual Meeting, Boston, MA, USA, November 2-6, **2025**.
- Montana Carlozo, Bridgette Befort, **Ning Wang**, Edward Maginn, and Alexander Dowling, "Bayesian Optimization for Nonlinear Model and Force Field Calibration", 2023 AIChE Annual Meeting, Orlando, FL, USA, November 5-10, **2023**.
- **Ning Wang**, Ryan Smith, Eliseo Marin-Rimoldi, Bridgette Befort, Alexander Dowling, Edward J. Maginn, "How Molecular Simulations Are Being Used to Phase out High Global Warming Potential Hydrofluorocarbon Refrigerants", 2022 AIChE Annual Meeting, Phoenix, AZ, USA, November 16, **2022**.
- Tianren Zhang, **Ning Wang**, Robert Riggleman, "Failure and mechanical properties of block copolymer thin films", Bulletin of the American Physical Society, Denver, CO, March 2, **2020**.

Teaching

Spring 2026	**Instructor**, CHEN 4341/MENG 5340 Special Topics, UT Tyler
Spring 2026	**Instructor**, CHEN 3320 Mass Transfer, UT Tyler
Fall 2025	**Instructor**, CHEN 2310 Introduction to Chemical Engineering, UT Tyler
Spring 2022	**Teaching Assistant**, CBE 30338 Chemical Process Control, Notre Dame
Fall 2021	**Teaching Assistant**, CBE 20255 Introduction to Chemical Engineering Analysis, Notre Dame
Spring 2021	**Teaching Assistant**, CBE 20258 Numerical and Statistical Analysis, Notre Dame
Fall 2020	**Teaching Assistant**, CBE 60553 Advanced Thermodynamics, Notre Dame
Spring 2020	**Teaching Assistant**, MSE 536 Electronic Properties of Materials, UPenn

Professional Service

External:

- Editorial Board Member, Journal of Ionic Liquids, Elsevier, October 2023 - present
- Journal reviewer, Polymer 2024; Journal of Chemical & Engineering Data 2024, 2025; ACS Sustainable Chemistry & Engineering 2025

Internal:

- Faculty Advisor, Society of Women Engineers, UT Tyler, August 2025 - present
- Faculty Committee Member for Graduate Students in Chemical Engineering (2), UT Tyler

Grants, contracts, and gifts

Industry gift, *POWER DREAM, Inc.*, 2025
Rising STARs Award, *The University of Texas System*, (09/2025-08/2028)

Honors

CBE Outstanding Paper Award in Molecular Simulations and Data Science, Notre Dame, 2024
Student Speaker Award, Notre Dame, 2023
Master's Scholar Award, UPenn, 2019