

Seyed Milad Hatamlee, PhD

RESEARCH INTERESTS

Molecular simulation of confined fluids and porous media; nanoscale heat and mass transport; machine-learning interatomic potentials; multiscale and thermodynamic modeling; carbon capture and energy materials; 2D materials and low-dimensional nano systems.

EDUCATION

PhD in Mechanical Engineering, GPA: 3.94/4.0 Jan. 2022 – May 2026

University at Buffalo, State University of New York, Buffalo, NY

Dissertation: Thermodynamics and Transport of Small Molecules under Nanoconfinement

Advisor: Dr. Jiaoyan Li

MS in Mechanical Engineering (Energy Conversion), GPA: 3.58/4.0 Sep. 2017 – Feb. 2020

Imam Khomeini International University (IKIU), Qazvin, Iran

Thesis: Heat Transport in 2D Structures of Carbon Nitride by Non-Equilibrium Molecular Dynamics

Advisor: Dr. Ali Rajabpour

BS in Mechanical Engineering Sep. 2013 – Sep. 2017

K.N. Toosi University of Technology (KNTU), Tehran, Iran

Thesis: Comparison of Ventilation Systems for Large Commercial Projects from an Economic Perspective

Advisor: Dr. Ali Behbahani Nia

RESEARCH EXPERIENCE

Research Assistant — University at Buffalo Jan. 2022 – May 2026

Multiscale/Multiphysics Theory and Simulation (MulTS) Laboratory

- Improved confined CO₂/hydrocarbon phase-equilibrium predictions by around 50% by integrating Monte Carlo simulation data with a modified Peng–Robinson EoS and temperature-dependent parameter optimization, enabling more accurate thermodynamic modeling for carbon capture and subsurface energy systems.
- Revealed a surface-wettability-controlled transition from flow enhancement to reduction in silica nanochannels, deviating up to about 200% from continuum predictions, by designing and simulating pressure-driven flow across 3 channel geometries and surface chemistries, providing molecular-scale design criteria for nanofluidic systems.
- Explained the competitive adsorption mechanism behind moisture-driven CO₂ capacity loss in zeolite 13X by simulating mixed CO₂/water transport at varying humidity levels, identifying site-blocking as the dominant molecular mechanism relevant to industrial CCS sorbent design.
- Enabled molecular-level CO₂/hydrocarbon phase prediction in nanopores, inaccessible to bulk EoS models, by building coupled MD/MC simulation workflows for binary mixture systems across a range of pressures, temperatures, and pore sizes, directly supporting carbon capture and enhanced oil recovery research.
- Reduced simulation turnaround time and minimized manual post-processing errors by building Python/Bash pipelines for LAMMPS and Towhee automation, HPC job scheduling, and data visualization.

Research Assistant — IKIU Feb. 2018 – Nov. 2021

Advanced Simulation and Computing Laboratory (ASCL)

- Quantified stress–strain response, Young's modulus, fracture strain, and deformation mechanisms across 8 MXene structures under tensile loading; identified how surface oxidation alters stiffness trends between carbide and nitride variants.
- Developed defect-concentration models for shear modulus and fracture strain in phosphorene, linking atomic-scale defects to mechanical degradation and predictive structural reliability assessment.
- Computed interfacial thermal conductance across 15 carbon-based heterostructures using NEMD, identifying localized interfacial vibrational modes as a stronger physics-based descriptor than phonon DOS overlap.

- Established density and Young's modulus as composite descriptors for thermal conductivity screening across 15 graphene polymorph systems, enabling faster structure–property evaluation without full simulation of every candidate.
- Trained machine-learning interatomic potentials using sparse DFT datasets and active learning, achieving higher accuracy in thermo-mechanical property prediction.

TEACHING EXPERIENCE

Course Instructor — MAE204 Thermodynamics I

Summer 2024

Department of Mechanical and Aerospace Engineering, University at Buffalo

- Independently designed course assessments and recitation sessions for 40+ undergraduate students.

Teaching Assistant — MAE385 Engineering Materials Lab

Spring 2023, 2024, 2025, 2026

Department of Mechanical and Aerospace Engineering, University at Buffalo

- Led 5 independent lab sections per semester across 4 years, guiding 200+ students per semester in hands-on materials characterization, mechanical testing, and microstructural analysis.

Teaching Assistant — MAE381 Engineering Materials

Fall 2022, 2023, 2024, 2025

Department of Mechanical and Aerospace Engineering, University at Buffalo

- Supported 300 students per semester through grading, office hours, and clarification of complex materials science concepts including crystal structure, defects, phase diagrams, and mechanical behavior.

PUBLICATIONS

Under Review

- Hatamlee SM, Li J. Molecular insights into water and CO₂ transport and adsorption in zeolite 13X. Under Review at Microporous and Mesoporous Materials, 2026.

Refereed Journal Articles

1. Hatamlee SM, Hoepfner M, Elmehlawy M, Lu M, Li Z, Li J. Modified Peng–Robinson equation of state for CO₂/hydrocarbon binaries under confinement based on Monte Carlo simulations. Accepted at Langmuir, 2026.
2. Hatamlee SM, Li J. Molecular dynamics study of water flow in silica nanochannels: transition from flow enhancement to reduction. Journal of Molecular Liquids, 2026 Jul 13:129795.
3. Xia Y, Liu J, Kancharla R, Li J, Hatamlee SM, Ren G, Semeykina V, Hamed A, Kane JJ. Insights into the 3D permeable pore structure within novel monodisperse mesoporous silica nanoparticles by cryogenic electron tomography. Nanoscale Advances, 5(11):2879–2886, 2023.
4. Ghasemi H, Hatamlee SM, Tirkolaei HK, Yazdani H. Biocementation of soils via enzyme induced carbonate precipitation: An integrated laboratory and molecular dynamics study. Biophysical Chemistry, 284:106793, 2022.
5. Hatamlee SM, Jabbari F, Rajabpour A. Interfacial thermal conductance between gold and SiO₂: A molecular dynamics study. Nanoscale and Microscale Thermophysical Engineering, 2022.
6. Hatamlee SM, Gordiz K, Rajabpour A. Lattice dynamics based descriptors for the interfacial heat transfer across 2D carbon-based nanostructures. Journal of Applied Physics, 2021.
7. Arabha S, Aghbolagh ZS, Ghorbani K, Hatamlee SM, Rajabpour A. Recent advances in lattice thermal conductivity calculation using machine-learning interatomic potentials. Journal of Applied Physics, 130(21):210903, 2021.
8. Hatamlee SM, Esfandiar A, Rajabpour A. Mechanical behaviors of titanium nitride and carbide MXenes: A molecular dynamics study. Applied Surface Science, 2021.
9. Hatamlee SM, Peer-Mohammadi H, Rajabpour A. Tuning shear mechanical properties and tensile strength anisotropy of monolayer black phosphorene: A molecular dynamics study. Materials Today Communications, 2020
10. Hatamlee SM, Rajabpour A, Volz S. Thermal conductivity of graphene polymorphs and compounds: from C₃N to graphdiyne lattices. Carbon, 161:816–826, 2020.

CONFERENCE PRESENTATIONS

- Hatamlee SM, Li J. Molecular dynamics study of water flow in silica nanochannels: surface wettability governs the transition from reduction to enhancement. American Physical Society, Division of Fluid Dynamics 78th Annual Meeting, Nov. 2025.
- Hatamlee SM, Li J. Modified Peng–Robinson equation of state for CO₂/hydrocarbon binaries under confinement based on Monte Carlo simulations. MUSE All-Hands Meeting, University of Utah, Salt Lake City, Jan. 2024.
- Hatamlee SM, Rajabpour A, Volz S. Thermal conductivity of graphene polymorphs and compounds: from C3N to graphdiyne lattices. 7th National Conference on Nanotechnology from Theory to Application, Jun. 2019.

TECHNICAL SKILLS

Simulation Methods: Molecular Dynamics (MD), Monte Carlo (MC), Density Functional Theory (DFT), ML Interatomic Potentials (MLIPs), Continuum Modeling, EoS Modeling

Software: LAMMPS, Towhee, VASP, Quantum ESPRESSO, OVITO, COMSOL, Abaqus

Programming: Python (NumPy, SciPy, Pandas, Matplotlib), Machine learning (PyTorch, Scikit-learn), MATLAB, Bash, LaTeX

Computing: High-Performance Computing (HPC), Linux, Git, automated simulation workflows

AWARDS, HONORS & CERTIFICATES

2025 Graduate Scholarship — J. & S. Niciszewska Mucha Endowed Scholarship, University at Buffalo (\$10,000)

2024 Leadership Grant — Council of Advocacy and Leadership Programming, UB (\$6,500)

2017 Ranked top 1% among 100,000+ participants, Iranian Undergraduate University Entrance Exam

2017 Ranked top 3% among 30,000+ participants, Iranian Master's Degree University Entrance Exam

2019 Certificate: A Not-so-brief Introduction to Molecular Biophysics, IPM, Tehran

2018 Certificate: Quantum Calculation using Quantum ESPRESSO, Sharif University of Technology

2018 Certificate: 1st Conference on the Computation of Nanostructures, Sharif University of Technology

SERVICE TO PROFESSION

Leadership	2024–2025 President, MAE Graduate Student Association, University at Buffalo
	2022–2024 President, Iranian Graduate Student Association (IGSA), University at Buffalo
Peer Review	2022, 2024 Journal of Applied Physics (3 manuscripts reviewed)

REFERENCES

Dr. Jiaoyan Li

Assistant Professor
Dept. of MAE, University at Buffalo
jiaoyan@buffalo.edu

Dr. Zachary Diermyer

Postdoctoral Research Associate
Idaho National Laboratory
Zachary.Diermyer@inl.gov

Dr. Jun Liu

Assistant Professor
Dept. of MAE, University at Buffalo
jliu238@buffalo.edu

Dr. Ali Rajabpour

Associate Professor, IKIU / IPM
Head, Advanced Simulation and Computing Lab
Rajabpour@ENG.ikiu.ac.ir