

Syed Milad Hatamlee

Ph.D. Candidate, University at Buffalo

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EDUCATION

Ph.D. in Mechanical Engineering, Jan. 2022 – Present

Department of Mechanical and Aerospace Engineering, University at Buffalo, Buffalo, NY, USA

Dissertation Title: Thermodynamics and Fluids Flow of Small Molecules under Nanoconfinement

Advisor: Dr. Jiaoyan Li

Master of Science in Mechanical Engineering (Energy Conversion), Sep. 2017 – Feb. 2020

Department of Mechanical Engineering, 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

Bachelor of Science in Mechanical Engineering, Sep. 2013 – Sep. 2017

Department of Mechanical Engineering, Khajeh Nasir Toosi University of Technology (KNTU), Tehran, Iran

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

Advisor: Dr. Ali Behbahani Nia

RESEARCH EXPERIENCE

Research Assistant, Jan. 2022 – Present

Department of Mechanical and Aerospace Engineering, University at Buffalo, Buffalo, NY, USA

Multiscale/Multiphysics Theory and Simulation (MulTS) Laboratory

Project:

- Investigated the confinement effects on thermodynamic behavior of small molecule mixtures (H_2O , CO_2 , CH_4 , C_7H_{16} , H_2) using molecular simulations, refining numerical predictions by up to 50% and resulting in a journal manuscript currently in preparation.
- Simulated nanoscale water flow to quantify deviations from classical predictions, providing critical insight into the nature of different behavior, and leading to an in-prep journal manuscript.

Research Assistant, Feb. 2018 – Nov. 2021

Department of Mechanical Engineering, Imam Khomeini International University, Qazvin, Iran

Advanced Simulation and Computing Laboratory (ASCL)

Project:

- Led molecular dynamics investigations into the mechanical and thermal properties of 2D materials, which resulted in multiple first-author publications and established new structure-property relationships.
- Developed machine learning-based interatomic potentials for new materials, reducing prediction error of thermal conductivity models by 20%.

TEACHING EXPERIENCE

Course Instructor, Summer 2024

Department of Mechanical and Aerospace Engineering, University at Buffalo

Course: MAE204 Thermodynamics 1

Responsibility: Designed Thermodynamics I course content and assessments; conducted recitations and mentored 50+ students, achieving 90% positive course evaluation ratings.

Teaching Assistant, Spring 2023/ Spring 2024 / Spring 2025

Department of Mechanical and Aerospace Engineering, University at Buffalo

Course: MAE385 Engineering Materials Lab

Responsibility: Independently led 4 lab sessions across 3 semesters for the Engineering Materials Lab, guiding 20+ students per semester and improving hands-on learning outcomes.

Teaching Assistant, Fall 2022/ Fall 2023/ Fall 2024

Department of Mechanical and Aerospace Engineering, University at Buffalo

Course: MAE381 Engineering Materials

Responsibilities: Grading, holding office hours, and clarifying complex concepts for 300 students each semester.

REFEREED JOURNAL ARTICLE PUBLICATION

Hatamlee SM, et.al., Molecular Dynamics Study of Water Flow in Silica Nanochannels: Surface Wettability Governs the Transition from Reduction to Enhancement (**Manuscript in Progress**)

Hatamlee SM, et.al., Modified Peng-Robinson Equation of State for CO₂/Hydrocarbon Binaries under Confinement Based on Monte Carlo Simulations (**Manuscript in Progress**)

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*. 2023;5(11):2879-86.

Ghasemi H, **Hatamlee SM**, Tirkolaei HK, Yazdani H. Biocementation of soils of different surface chemistries via enzyme induced carbonate precipitation (EICP): An integrated laboratory and molecular dynamics study. *Biophysical Chemistry*. 2022 May 1;284:106793.

Hatamlee SM, Jabbari F, Rajabpour A. Interfacial thermal conductance between gold and SiO₂: A molecular dynamics study. *Nanoscale and Microscale Thermophysical Engineering*. 2022 Apr 28:1-2.

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 Sep.

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*. 2021 Dec 7;130(21):210903

Hatamlee SM, Esfandiar A, Rajabpour A. Mechanical behaviors of titanium nitride and carbide MXenes: A molecular dynamics study. *Applied Surface Science*. 2021 Jul 16:150633.

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 Nov 2:101796.

Hatamlee SM, Rajabpour A, Volz S. Thermal conductivity of graphene polymorphs and compounds: from C₃N to graphdiyne lattices. *Carbon*. 2020 May 1; 161:816-26.

CONFERENCE PRESENTATION

Thermal conductivity of graphene polymorphs and compounds: from C₃N to graphdiyne lattices. 7th National Conference on Nanotechnology from theory to application, Date: 06/15/2019

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, Date: 01/25/2024

AWARDS, HONORS, CERTIFICATE

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

Leadership Grant: \$6,500 from the Council of Advocacy and Leadership Programming for IGSA (2024)

Ranked the top 1% among more than 100,000 participants in the Iranian undergraduate university entry exam.

Ranked the top 3% among more than 30,000 participants in the Iranian master's degree university entry exam

Certificate: **A Not-so-brief Introduction to Molecular Biophysics**, Date: 04/28/2019
Institute for Research in Fundamental Sciences (IPM), Tehran, Iran.

Certificate: **Quantum calculation using Quantum Espresso**, Date: 07/08/2018
Sharif University of Technology, Tehran, Iran.

Certificate: **1st conference on the computation of nanostructures** , Date: 07/08/2018
Sharif University of Technology, Tehran, Iran.

SERVICE TO PROFESSION

Journal Manuscript Review

Journal of Applied Physics, Year: 2022, and 2024 (3 reviews)

Leadership Position

-Iranian Graduate Student Association at UB, Year: 2022-2024

President of the club for two consecutive years.

-Mechanical and Aerospace Engineering Graduate Student Association at UB, Year: 2024-2025

President of the club.

PROFESSIONAL SKILLS

Computational Methods:

Molecular Dynamics (MD), Monte Carlo (MC), Density Functional Theory (DFT), AI/ML, Machine Learning Interatomic Potentials (MLIPs), Continuum Modeling

Softwares and packages

LAMMPS, VASP, Quantum ESPRESSO, GULP, Towhee, COMSOL, Abaqus, OVITO, VMD, Solid Works

Programming & Data Science:

Python, MATLAB, Linux/Bash, High-Performance Computing (HPC)