ZARIF AHMAD RAZIN BHUIYAN

Raleigh, NC zrazinb@ncsu.edu
www.abzarif.com ORCID: 0000-0002-2977-2392 Google Scholar

EDUCATION

North Carolina State University (NCSU), Raleigh, NC
PhD in Mechanical Engineering | GPA: 4.00/4.00 *Aug 2024 – present*
MS in Mechanical Engineering | GPA: 4.00/4.00 *Aug 2026*

Bangladesh University of Engineering & Technology (BUET), Dhaka
BSc. in Mechanical Engineering | CGPA: 3.76/4.00 *May 2022*

RESEARCH EXPERIENCE

Graduate Research Assistant, NCSU *Aug 2024 – present*
Nano-scale Thermal Transport Lab | Advisor: Dr. Jun Liu

- **Organic Solar Cell:** Reparameterized classical molecular dynamics (MD) force field using quantum mechanical (QM) calculations and unsupervised machine learning to analyze Y6 molecule dimers.
- **Perovskite Materials:** Investigated ultra-low thermal conductivity mechanisms in perovskites through equilibrium MD simulations.
- **Polymer Composites:** Modeled interfacial thermal resistance of PU-THDBT polymer filler-matrix composites using non-equilibrium molecular dynamics (NEMD) simulations and vibrational density of states analysis.
- **Glass Transition:** Investigated semicrystalline polymer thermal transport around the glass transition temperature using enhanced Monte Carlo and NEMD simulations.
- **Chiroptical Sensors:** Modeled enantioselective glucose adsorption on twisted aligned carbon nanotubes (CNTs) for ultrasensitive chiroptical sensing.
- **Soft Matter Modeling:** Developing molecular models to predict the structure and properties of soft materials.

Course Project

- **Machine Learned Potentials:** Developed a deep neural network (DNN) machine-learned potential for silicon to replace traditional empirical force fields.

Undergraduate Researcher, BUET *Apr 2021 – Apr 2022*
Advisor: Dr. A.K.M. Monjur Morshed

- **Nano-confined Liquids:** Analyzed specific heat and thermal conductivity of confined liquid argon to determine the effect of surface wettability.

TEACHING EXPERIENCE

Course Lectures, NCSU *Fall 2025*

- Delivered two lectures on molecular dynamics simulations with LAMMPS in MAE 720: Molecular Level Modeling for Engineering Applications, taught by Dr. Jun Liu.
  – *Lecture guide: abzarif.com/resources/md-lammps-guide*

Lecturer, Sonargaon University (SU), Dhaka *May 2023 – Jun 2024*

- Taught undergraduate theory courses: ME 321: Fluid Mechanics I, ME 323: Fluid Mechanics II, and ME 349: Mechanics of Machinery I.

Teaching Assistant, BUET *Nov 2022 – Apr 2023*

- Assisted in sessional (lab) courses: ME 160: Mechanical Engineering Drawing, ME 302: Heat Transfer Sessional, and ME 310: Heat Transfer Equipment Design.

PUBLICATIONS

Journal Articles

1. Z. Wang†, L. Yan†, A. Negi†, Q. Wang†, **Z.A.R. Bhuiyan**, X. Zhong, A.H. Comstock, S. Mukherjee, Y. Yu, C. Yang, A. Jouneghaninaseri, S. Khan, T. Wang, S. Raza, J. Hu, Y. Nabei, X. Gu, H. Shao, M. Liu, Q. Tu, H. Ade, J. Zhou*, D. Sun*, W. You*, and J. Liu*, "Extremely Low Thermal Conductivity in Rigid Layered Hybrid Perovskites", *Science Advances* 12 (38) (2026): eaee5269.
2. H. Worden†, M. Chandra†, Y. Zhou†, **Z.A.R. Bhuiyan**, M. Cheng, K. Munusamy, D. Nghiem, W. Hu, W. Yan, S. Wu, R. Li, Z. Jiang, A. Chatterji, S. Zhang, I.N. Ivanov, J. Chen, J.C. Lasseter, M. Jin, D. Abitagaoglu, Q. Tu, T. Emrick, J. Liu, and Y. Xu*, "Suppressing Thermal Transport in Nonporous Polymer Hybrids by Limiting Thermally Accessible Vibrational Modes", *Materials Horizons* 13 (12) (2026): 5876–5887. (Selected as the Inside Front Cover)
3. H. Xie, J. Fan, **Z.A.R. Bhuiyan**, S. Raza, M. Mohammadi, C. Guo, Y. Wang, J. Liu, and W. Gao*, "Ultrasensitive Enantioselective Chiroptical Sensing with Large-Area Twisted Aligned Carbon Nanotube Films", *ACS Nano* (2026).
4. P. Das†, **Z.A.R. Bhuiyan**†, A.K.M.M. Morshed, and T.C. Paul, "Thermal Properties of Liquid Entrapped Between Hybrid Wettability Surface", *Computational Materials Science* 244 (2024): 113232.
5. A.K.M.M. Morshed†, P. Das†, and **Z.A.R. Bhuiyan**†, "Effect of Surface Wettability on Specific Heat Capacity of Nano-Confined Liquid", *Journal of Molecular Liquids* 383 (2023): 122115.

Under Review

6. S.C. Yelishala, **Z.A.R. Bhuiyan**, H. Zhou, Y. Ding, A.J.H. McGaughey, R.C. Hayward, J. Liu*, and L. Cui*, "Giant Thermal Conductivity Switching via Glass Transition in Semicrystalline Polymers", *under review* (2026).

† Authors contributed equally; * Corresponding author

SKILLS

- **Molecular Dynamics & QM:** LAMMPS, AMBER, VASP, Gaussian (HF, DFT)
- **Machine Learning & Data Science:** PyTorch, scikit-learn, Pandas
- **Programming Languages:** Python (fluent), MATLAB (fluent)
- **Computing & OS:** High-Performance Computing (HPC), Linux (Ubuntu), Shell Scripting

AWARDS AND SCHOLARSHIPS

- **Provost Doctoral Fellowship** *Aug 2024*
  – Awarded by North Carolina State University
- Graduation with **Honors** *May 2022*
  – Awarded by BUET for graduation with CGPA ≥ 3.75
- **University Merit List Scholarship** *All academic years*
  – Awarded by BUET for merit position in the top 20% of the class

REFERENCES

Available upon request.