Fakhrul Hasan Bhuiyan

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Education

Ph.D. in Mechanical Engineering — *Aug 2019 - Aug 2024*
University of California Merced — *Merced, CA*
CGPA: 3.97/4.00

B.Sc. in Mechanical Engineering — *Jul 2014 - Oct 2018*
Bangladesh University of Engineering and Technology — *Dhaka, Bangladesh*
CGPA: 3.51/4.00

Research & Work Experience

Postdoctoral Researcher — *Sep 2024 - Current*
Computational Science Division, Argonne National Laboratory — *Lemont, IL*

- Performed computational research on molten salts, transition metal complexes, and electrochemical systems using density functional theory (DFT), molecular dynamics (MD), data analysis, and machine learning (ML)
- Developed machine-learned interatomic potentials (MLIPs) using the MACE framework with an active learning workflow to simulate molten salts containing iron, lithium, potassium, and/or chlorine
- Created a graph construction and graph neural network training pipeline to model the reduction potential of transition metal complexes, achieving state-of-the-art performance with an error margin of about ± 0.2 V
- Designed and optimized scalable workflows for managing and executing thousands of DFT calculations and MD simulations, accelerating the development of MLIPs on ALCF supercomputers
- Crafted a modern, user-friendly web app to visualize the NIST SRD 46 database, streamlining access to key data on a wide range of ligands for the chemistry and electrochemistry communities
- Secured $50k in seed funding as a co-PI to develop a visual language model for structured and critical analysis of cyclic voltammetry images

Research Assistant — *Jan 2020 - Aug 2024*
Dept. of Mechanical Engineering, University of California Merced — *Merced, CA*

- Performed computational research on mechanical systems involving surfaces, lubricants/additives, and nanomaterials using reactive MD simulations and high-performance computing (HPC)
- Conducted nine collaborative research projects, published three first-author papers in peer-reviewed journals, and gave eight oral presentations at four international conferences and three research seminars
- Developed a computational method of quantifying molecular-level deformation using statistical analysis
- Developed in-house Python modules to store, analyze, and interpret simulation and modeling data 2x faster
- Led the simulation team sub-group in the lab and mentored fellow graduate students on atomistic simulations and Python scripting

Visiting Scholar — *Jan 2022 - Jan 2022*
Dept. of Materials Science and Engineering, The Pennsylvania State University — *State College, PA*

- Obtained hands-on training on ball-on-flat sliding experiments using a tribometer, performed optical microscopy, and scanning electron microscopy (SEM) to characterize samples and surfaces
- Conducted chemical analysis and characterization of surfaces using energy-dispersive X-ray spectroscopy (EDX), and Raman spectroscopy

Teaching Assistant for Engineering Computing — *Aug 2019 - Dec 2019*
School of Engineering, University of California Merced — *Merced, CA*

- Led Python and MATLAB discussion lab of 25 students, graded problem sets and class exercises, and helped students in solving class and quiz problems

Industrial Trainee — *Mar 2018 - Apr 2018*
Pragoti Industries Ltd — *Chattogram, Bangladesh*

- Hands-on experience in statistical process control (SPC) of automobile parts, Design of Experiments (DOE), material handling, machining, and quality control processes

Publications (Journal Papers)

10. Faiyad, A., Bhuiyan, F. H., Vellore, A., Johnson, D., Kennett, A., & Martini, A. (2024). Mechanisms of MoS_2 dry film lubricant behavior at low temperatures. Friction, 2025, 13(4): 9441020.
9. Cobeña-Reyes, J., Bhuiyan, F. H., & Martini, A. (2024). Atomistic simulations of mechanically activated reactions for oxygen release from polymers. RSC Mechanochemistry.
8. Li, Y. S., Bhuiyan, F. H., Kim, S. H., & Martini, A. (2024). Elucidating Tribochemical Reaction Mechanisms: Insights into Tribofilm Formation from Adsorbates Coupled with Tribochemical Substrate Wear. RSC

Mechanochemistry.

7. Bhuiyan, F. H., Li, Y. S., Kim, S. H., & Martini, A. (2024). Shear-Activation of Mechanochemical Reactions Through Molecular Deformation. Scientific Reports, 14, 2992.
6. Ogbomo, E., Bhuiyan, F. H., Latorre, C. A., Martini, A., & Ewen, J. P. (2024). Effects of Surface Chemistry on the Mechanochemical Decomposition of Tricresyl Phosphate. Physical Chemistry Chemical Physics, 26(1), 278-292.
5. Chen, L., Yan, W., Bhuiyan, F. H., Tang, C., Jiang, Y., Jang, S., Liu, Y., Wu, J., Wang, W., Wang, Y., Zheng, J., Martini, A., Qian, L., & Kim, S. H. (2023). Understanding and Preventing Lubrication Failure at the Carbon Atomic Steps. Small, 2301515.
4. Li, Y. S., Jang, S., Bhuiyan, F. H., Martini, A., & Kim, S. H. (2023). Molecular Structure and Environment Dependence of Shear-driven Chemical Reactions: Tribopolymerization of Methylcyclopentane, Cyclohexane and Cyclohexane on Stainless Steel. Tribology Letters, 71(2), 49.
3. Bhuiyan, F. H., Li, Y. S., Kim, S. H., & Martini, A. (2023). Shear-Activated Chemisorption and Association of Cyclic Organic Molecules. Faraday Discussions, 241, 194-205.
2. Bhuiyan, F. H., Kim, S. H., & Martini, A. (2022). Reactive Molecular Dynamics Simulations of Thermal and Shear-driven Oligomerization. Applied Surface Science, 591, 153209.
1. Khajeh, A., Bhuiyan, F. H., Mogonye, J. E., Pesce-Rodriguez, R. A., Berkebile, S., & Martini, A. (2021). Thermal Decomposition of Tricresyl Phosphate on Ferrous Surfaces. The Journal of Physical Chemistry C, 125(9), 5076-5087.

Skills

Programming Languages

- Python, LAMMPS, VASP, Bash scripting, Shell scripting, LaTeX, HTML

Computational Techniques

- Molecular dynamics, ReaxFF, Density functional theory, Nudged elastic band calculations, HPC, Big data analysis, Data scraping

Machine Learning Techniques

- ML-based interatomic potential, Graph neural networks, Active Learning, Supervised learning, Large language models (fine-tuning and inference)

Awards, Honors, & Fundings

Argonne Training Program on Extreme-Scale Computing (ATPESC) Attendee *Summer 2025*
Argonne National Laboratory

Seed Funding to Develop Language Models for Electrochemistry ($\$50k$) *Summer 2025*
Argonne National Laboratory

Graduate Dean's Dissertation Fellowship *Spring 2024*
Division of Graduate Studies, University of California Merced

Grad Slam Finalist *Spring 2023*
Division of Graduate Studies, University of California Merced

GRAD-EXCEL Peer Mentor Fellowship *Spring 2023*
Division of Graduate Studies, University of California Merced

ME Spring 2023 Travel Fellowship *Spring 2023*
School of Engineering, University of California Merced

ME Bobcat Travel Fellowship *Spring 2022*
School of Engineering, University of California Merced

Research Scholarship *Jan 2022*
Society of Tribologists and Lubrication Engineers (STLE) Northern California Section

Bobcat Fellowship *Spring 2022*
School of Engineering, University of California Merced

ME Travel Award *Spring 2020*
School of Engineering, University of California Merced

Leadership & Teamwork Experience

Team Mentor *May 2025 - May 2025*
ALCF INCITE GPU Hackathon, Argonne National Laboratory *Lemont, IL*

- Assisted participating teams with coding support, providing guidance on accessing ALCF supercomputers, and helping with software setup and configuration.

Company Outreach Member *May 2025 - Oct 2025*
Postdoc Research and Career Symposium, Argonne National Laboratory *Lemont, IL*

- Coordinated outreach and communication with multiple multiple companies to secure their registration and participation in the 2025 Postdoc Research and Career Symposium

Founding & Executive Member *May 2022 - Aug 2024*
Bangladesh Student Association, University of California Merced *Merced, CA*

- Edited and reviewed grant applications, collected members, documented the club constitution, and organized meetings and events

Presider of the COMP Quantum Mechanics session *Mar 2024 - Mar 2024*
American Chemical Society Spring 2024 Conference *Long Beach, CA*

- Conducted the "COMP Quantum Mechanics" session at the ACS Spring 2024 Conference, introduced the speakers, and led the Q/A sessions

Session Chair for the Lubrication Fundamentals IV *May 2023 - May 2023*
Society of Tribologists and Lubrication Engineers (STLE) 2023 Annual Meeting & Exhibition *Long Beach, CA*

- Conducted the "Lubrication Fundamentals IV: Polymers" session at the STLE 2023 Annual Meeting & Exhibition, introduced the speakers, and led the Q/A sessions and the business meeting

Grad-Excel Peer Mentor *Aug 2022 - May 2023*
Division of Graduate Studies, University of California Merced *Merced, CA*

- Mentored first-year graduate students, helped them with research and coursework and monitored their overall well-being to ensure their proper adjustment to graduate school

Oral Presentations & Posters

10. Development and Application of Machine Learning Interatomic Potentials at Scale for Steelmaking Research *May 2025*
Oral presentation, Center for Nanoscale Material - Theory and Modeling Seminar

9. Hour of Code! *Dec 2024*
Oral presentation, Loyola Academy Wilmette

8. Shear-activation of mechanochemical reactions through molecular deformation *Mar 2024*
Oral presentation, American Chemical Society Spring 2024

7. Molecular Mechanisms of Tribochemical Reactions: Reactive Molecular Dynamics Simulations of Cyclic Organic Molecules *May 2023*
Poster presentation, STLE 2023 Annual Meeting & Exhibition

6. Molecular Mechanisms of Tribochemical Reactions: Reactive Molecular Dynamics Simulations of Cyclic Organic Molecules *May 2023*
Oral presentation, STLE 2023 Annual Meeting & Exhibition

5. Molecular Mechanisms of Tribochemical Reactions: Reactive Molecular Dynamics Simulations of Cyclic Organic Molecules *Oct 2022*
Oral presentation, Web Seminar Series on Tribology

4. Simulating Tribochemical Reactions with Molecular Dynamics and Improving Performance of Lubricant Additives *May 2022*
Oral presentation, STLE Northern California Section Meeting

3. Reactive Molecular Dynamics Simulations of Thermal and Shear-Driven Tribopolymerization *May 2022*
Oral presentation, STLE Annual Meeting & Exhibition

2. Reactive Molecular Dynamics Simulations of Thermal and Shear-Driven Oligomerization *Mar 2022*
Poster presentation, American Chemical Society Spring 2022

1. Reactive Molecular Dynamics Simulations of Tribochemical Reactions *Jan 2022*
Invited oral presentation, Dr. Seong Kim's research group at The Pennsylvania State University, State College, PA

Research Projects

ML-Forcefields for Molten Salts *Sep 2024 - Current*
Developing machine learning-based forcefields for accurate molecular dynamics simulations of molten salts containing transition metals.

Graph Neural Networks for Modeling Redox Potential of Metal Complexes *Jan 2025 - Current*
Creating graph neural network models to predict redox potentials of transition metal complexes from the tmQM dataset for rapid screening purposes.

Generative Large Language Model for Tribology *June 2023 - Aug 2024*
Fine-tuning the open LLama 13B parameter model on a custom-made dataset consisting of tribology literature for summarizing, question-answering, and hypothesis-generation tasks.

Temperature-Dependent Wear Life of MoS_2 Dry Film Lubrication *Oct 2022 - Aug 2024*
Conducting reactive MD simulations of MoS_2 dry film coatings to study the friction and wear behavior at cryogenic and room temperatures and explain the temperature-dependent wear life of MoS_2 coatings, in collaboration with ball-on-flat tribometer experiments.

Mechanochemical Reactions of Organic Compounds and Commercially Used Antiwear Additives *Jan 2021 - Current*
Using reactive MD simulations and data analysis techniques to study the nanoscale mechanisms of mechanochemical reactions of simple organic molecules and commercially used antiwear additives, in collaboration with ball-on-flat tribometer experiments.

Friction on Graphite Step-Edges *Jul 2021 - Jul 2022*
Studied the friction and chemical reactivity on graphite using reactive MD simulations to identify different defects on graphite, in collaboration with atomic force microscopy experiments.

Structure of Adsorbed Water *Aug 2020 - Feb 2021*
Analyzed the structure of adsorbed water layer on silica using reactive MD simulations and revealed a transition from water to ice-like structure near the surface.

Thermal Decomposition of Phosphorous-Based Lubricant Additives on Ferrous Surfaces *Sep 2019 - Dec 2020*
Investigated the thermal decomposition reaction mechanisms of a commercially used antiwear additive, and the difference in reactivity of three isomers to elucidate the working principles of the antiwear additive, in collaboration with temperature-programmed reaction spectroscopy and gas chromatography-mass spectroscopy.

Fully Automated Large-scale Juice Maker *Aug 2016 - Dec 2016*
3D designed a prototype, produced machine parts through cast molding, and assembled parts and materials to create a fully automated juice maker.

Research Interests

- Computational research on mechanical, chemical, and biological problems
- Machine learning-based potentials for computational simulations
- Data science and Machine learning
- Mechanochemical reactions
- Fundamental mechanisms of nanomaterials
- 2-D nanomaterials
- Friction, wear, and lubrication

References

- **Dr. Ashlie Martini** (amartini@ucmerced.edu)
  - Professor and Chair of Mechanical Engineering, University of California, Merced
- **Dr. Seong H. Kim** (shk10@psu.edu)
  - Professor of Chemical Engineering and Materials Science and Engineering, Pennsylvania State University
- **Dr. Arash Khajeh** (arash.khajeh@gmail.com)
  - Research Scientist, Toyota Research Institute