Abrar Faiyad

PhD candidate, Mechanical Engineering, UC Merced · Merced, California, USA

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SUMMARY

Trains models of atomic interactions on quantum calculations and tests where they work in molecular dynamics simulations of molten salts, lubricants, and electrode interfaces.

EDUCATION

University of California, Merced Jan 2023 – present

Ph.D., Mechanical Engineering · GPA 3.93 / 4.00. Advisor: Prof. Ashlie Martini.

University of California, Merced May 2026

M.S., Mechanical Engineering · GPA 3.93 / 4.00.

Bangladesh University of Engineering and Technology (BUET) Feb 2017 – May 2022

B.Sc., Mechanical Engineering · First-author PCCP paper as an undergraduate.

RESEARCH EXPERIENCE

Guest Facility User · Argonne National Laboratory · Center for Nanoscale Materials Fall 2026 – present

- Train and fine-tune MACE, MACE-RSGA, and eSEN models for platinum–water interfaces.
- Compare reaction barriers and solvent structure against DFT and ab initio MD.
- Use active learning to add the atomic environments the models are missing.

Research Aide Technical – PhD · Argonne National Laboratory · Computational Science Division

Mar 2026 – Aug 2026

- Fine-tuned universal MACE potentials for molten LiCl–$FeCl_2$ with multi-head replay and LoRA. This removed an unphysical Fe–Fe clustering artifact inherited from solid-state training data.
- Validated liquid structure against high-energy X-ray diffraction (mean R-factor 0.034) across composition and temperature.
- Automated DFT frame generation for labeled training data across molten-salt compositions on ALCF systems.
- Built an uncertainty-biased active-learning loop: bias forces push MD toward uncertain configurations, which are DFT-labeled and added to training.
- Computed excess thermodynamic properties and the LiCl–KCl phase diagram with Kirkwood–Buff theory on ML-driven MD.
- Trained and benchmarked MACE foundation models on the Open Catalyst 2025 (OC25) dataset at Aurora scale. Built agentic workflows that set up data generation and fine-tuning from plain-language instructions.

Visiting Scholar · NASA Jet Propulsion Laboratory Mar 2025

- Ran tribometry of MoS_2 dry-film coatings across temperatures.
- Fed the observations into the low-temperature wear simulations.

Graduate Student Researcher · Martini Research Group · University of California, Merced

Jan 2023 – present

- Fine-tuned a MACE model for MoS_2–N_2 with LoRA and automated DFT data. Validation energy RMSE fell from 76.0 to 9.2 meV/atom.
- Benchmarked Meta's universal UMA potential against DFT for 25 MoS_2 dopants and published the workflow as open source (JCTC 2026).
- Trained DeepMD potentials for ions at solid–liquid electrochemical interfaces.
- Co-originated, and helped benchmark the ML potential for, a study of ion adsorption on gold (JCP 2026).
- Ran fracture, water-adsorption, and sliding simulations that explain cold-temperature failure of MoS_2 lubricants (Friction 2025).

Research Assistant · Motalab Lab · BUET Jun 2022 – Dec 2022

- Related cooling rate and microstructure to void nucleation and cyclic response.
- Mentored undergraduates in simulation and analysis. The work led to peer-reviewed papers on solder, CdTe nanowires, and printed Inconel.

PUBLICATIONS

1. **A. Faiyad**, A. Martini. Machine Learning Interatomic Potentials Enable Molecular Dynamics Simulations of Doped MoS_2. *Journal of Chemical Theory and Computation* 22(5), 2574–2585 (2026). doi:10.1021/acs.jctc.5c02004
2. F. Roncoroni, **A. Faiyad**, Y. Li, T. Ye, A. Martini, D. Prendergast. Deriving Effective Electrode–Ion Interactions from Free-Energy Profiles at Electrochemical Interfaces. *The Journal of Chemical Physics* 164(8), 084702 (2026). doi:10.1063/5.0321463
3. **A. Faiyad**, F. H. Bhuiyan, A. Vellore, D. A. Johnson, A. Kennett, A. Martini. Mechanisms of MoS_2 Dry Film Lubricant Behavior at Low Temperatures. *Friction* 13(4), 9441020 (2025). doi:10.26599/FRICT.2025.9441020
4. **A. Faiyad***, D. Miliate*, S. Leventini, J. R. Lince, A. Martini. Temperature-Dependent Friction, Wear, and Life of MoS_2 Dry Film Lubricants for Space Mechanisms: A Comprehensive Review. *Tribology Letters* 73(4), 114 (2025). doi:10.1007/s11249-025-02052-6
5. S. Fardin, M. J. Moresalein, M. Motalab, **A. Faiyad**, R. Paul. Effects of Ultra-High Cooling Rates on the Tensile and Cyclic Stress–Strain Behavior of Nanoscale Solder Materials. *Journal of Electronic Materials* (2025). doi:10.1007/s11664-025-12048-6
6. M. N. Azad, S. Zafar, **A. Faiyad**, H. S. Sim, S. L. Hong. Atomistic Study of Selenium Doping Effects on the Mechanical Properties of Zinc-Blende and Wurtzite CdTe Nanowires. *Computational Materials Science* 246, 113410 (2025). doi:10.1016/j.commatsci.2024.113410
7. S. R. Romero Garcia, **A. Faiyad**, A. Martini. Modeling Sputtering Deposition of MoS_2: Effect of Ni Doping on Nanostructure and Tribological Properties. *Computational Materials Science* 244, 113229 (2024). doi:10.1016/j.commatsci.2024.113229
8. T. Islam, M. S. A. Aziz, M. Motalab, **A. Faiyad**. Atomistic Study on the Cooling Rate Induced Mechanical Properties Variations in Additively Manufactured Inconel-718. *ASME IMECE 2023* Paper IMECE2023-114456 (2023). doi:10.1115/IMECE2023-114456
9. S. M. A. A. Alvi, **A. Faiyad**, M. A. M. Munshi, M. Motalab, M. M. Islam, S. Saha. Cyclic and Tensile Deformations of Gold–Silver Core–Shell Systems Using Newly Parameterized MEAM Potential. *Mechanics of Materials* 169, 104304 (2022). doi:10.1016/j.mechmat.2022.104304

10. **A. Faiyad**, M. A. M. Munshi, M. M. Islam, S. Saha. Deformation Mechanisms of Inconel-718 at the Nanoscale by Molecular Dynamics. *Physical Chemistry Chemical Physics* 23(17), 10650–10661 (2021). doi:10.1039/D0CP06614A

Under review and in preparation

1. **A. Faiyad**, F. H. Bhuiyan, J. Guo, C. J. Benmore, Á. Vázquez-Mayagoitia. Elucidating Bulk Structure, Transport Properties, and Chain Formation in Molten LiCl–$FeCl_2$: A Temperature and Composition Analysis. *Under review*.
2. **A. Faiyad**, et al.. Fine-tuning a Foundation Interatomic Potential to Investigate Nitrogen-Dependent Structural Evolution in MoS_2. *In preparation*.
3. **A. Faiyad**, et al.. Uncertainty-Biased Active Learning of MACE Interatomic Potentials for Complex Interfaces. *In preparation*.
4. **A. Faiyad**, et al.. Thermodynamic Properties and Phase Diagram of Molten LiCl–KCl from ML Interatomic Potentials and Kirkwood–Buff Theory. *In preparation*.

SKILLS

Machine-learning potentials: MACE, UMA (fairchem), eSEN, DeepMD-kit, LoRA fine-tuning, Multi-head replay, Active learning, Uncertainty estimation

Simulation: LAMMPS, ASE, VASP, Quantum ESPRESSO, ReaxFF, EAM / MEAM, Metadynamics, Free-energy profiles

Data & code: Python, PyTorch, NumPy, SciPy, pandas, scikit-learn, Matplotlib, MATLAB

HPC & workflow: ALCF Aurora, ALCF Polaris, Slurm, PBS, MPI, GPU scaling, High-throughput DFT, Agentic workflows

Analysis & visualization: OVITO, VMD, Kirkwood–Buff theory, RDF / structure factor, MSD / diffusion, Parity & error analysis

PRESENTATIONS

Effects of flake size on MoS_2 dry film lubricants at low temperature May 2025
Oral · STLE Annual Meeting & Exhibition, Atlanta, GA

Low-temperature mechanisms of MoS_2 June 2024
Oral + poster · Gordon Research Conference (Tribology), Bates College, ME

LEADERSHIP & PROFESSIONAL DEVELOPMENT

Argonne Training Program on Extreme-Scale Computing (ATPESC) July 2026
Selective two-week program on programming and scaling scientific applications on leadership-class HPC systems.

Multiscale Mechanical Modeling and Research Network, BUET 2021 – present
Vice president (Jun 2021 – May 2022), now mentor. Organized 12 public webinars on computational mechanics and mentored students learning MD, which led to several peer-reviewed papers.

Peer reviewer 2024 – 2025
Reviewer certificates issued February 2024 and October 2025.