

## Research Interest

Computational Materials Science, Molecular and Multi-scale Modeling, Machine Learning, Deep Learning, Density Functional Theory, Metamaterials.

## Education

Ph.D. in Mechanical Engineering (Expected) September, 2028  
Specialization: **Molecular and Multi-scale Modeling, Nanomaterials**  
University of Rochester, United States. GPA: 4/4

MS in Mechanical Engineering 09/01/2023  
Specialization: **2D Materials, Molecular Simulations**  
University of Massachusetts, Amherst, United States. GPA: 3.9/4 (overall)

B.Sc. in Mechanical Engineering 07/2014 - 10/2018  
Specialization: **Molecular Modeling, Nanotechnology**  
Bangladesh University of Engineering and Technology, Bangladesh. GPA: 3.71/4 (overall)

## Professional Experience

Journal Article Reviewer 08/2024 - Present  
Nature Communications, Nature Publishing Group, **ORCID**


Research & Teaching Assistant 09/2023 - Present  
Department of Mechanical Engineering,  
University of Rochester, Rochester, NY

Research & Teaching Assistant 01/2021 - 08/2023  
Department of Mechanical and Industrial Engineering,  
University of Massachusetts, Amherst, MA

HVAC Design Coordinator and Project Supervisor 07/2019 - 01/2021  
MEP Design Studio, Dhaka, Bangladesh


Paid Co-op Internship, Engineering Division 03/2018 - 04/2018  
Eskayef Pharmaceuticals Ltd., Dhaka, Bangladesh

## Awards & Achievements

 MIE Departmental Fellowship, University of Massachusetts Amherst 2021

 University Dean's award for academic excellence in B.Sc. 2016-2018

 University Merit and Technical scholarships for academic excellence in B.Sc. 2014-2016

 National Education Board Scholarship for securing top 100 amongst 230,000 candidates 2011

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## Publications

### Journal Articles (peer-reviewed)

- J1.** Mostafa, A., Vu, L., Guo, Z., Shargh, A. K., Dey, A., Askari, H., Abdolrahim, N., “Phase-transformation assisted twinning in molybdenum nanowires,” *Computational Materials Science*, vol. 244, p. 113 273, 2024.
- J2.** Mostafa, A., Ramasubramaniam, A., Maroudas, D., “Thermal conductivity of 2D diamond superstructures in interlayer-bonded twisted bilayer graphene,” *Applied Physics Letters*, vol. 122, no. 13, 2023.
- J3.** Mostafa, A., Weerasinghe, A., Ramasubramaniam, A., Maroudas, D., “Response of interlayer-bonded bilayer graphene to shear deformation,” *Journal of Applied Physics*, vol. 134, no. 15, 2023.

### Journal Articles (under preparation)

- J4.** Li, F., Mostafa, A., Zimmerman, J., Liang, Z., Klinger, L., Yeom, J., Janczak-Rusch, J., Abdolrahim, N., Rabkin, E., “Solid-state dewetting of co-sputtered thin Mo-Cu films accompanied by phase separation,” 2024.
- J5.** Qian, S., Mostafa, A., Li, F., Rabkin, E., Abdolrahim, N., “Orientation-dependent phase transformation in Molybdenum nanowires under uniaxial and bi-axial bending deformation,” 2024.

### Conference Proceedings

- C1.** Mostafa, A., Motalab, M., Faiyaz, A. R., Paul, R., “Uniaxial and cyclic stress-strain behavior of lead-free solders at nanoscale,” in *AIP Conference Proceedings*, AIP Publishing, vol. 2324, 2021.

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## Presentations

A. Mostafa, L. Vu, F. Li, A. Dey, H. Askari, E. Rabkin, and N. Abdolrahim, “Novel Methods for Phase-Transformation-Assisted Twinning in Molybdenum Nanomaterials: Simulation and Experimental Study”, *ASME International Mechanical Engineering Congress and Exposition (IMECE) 2024, Portland, OR (Scheduled)*.

S. Qian, A. Mostafa, F. Li, E. Rabkin, and N. Abdolrahim, “Influence of Non-Uniaxial Bending on Twinning and Phase Transformation in Molybdenum Nanowires”, *ASME International Mechanical Engineering Congress and Exposition (IMECE) 2024, Portland, OR (Scheduled)*.

A. Mostafa, L. Vu, F. Li, A. Dey, H. Askari, E. Rabkin, and N. Abdolrahim, “Atomistic insights on orientation-dependent deformation mechanisms in Molybdenum: Single-crystal nanowires and polycrystals”, *TMS Annual Meeting & Exhibition 2025, Las Vegas, NV (Scheduled)*.

F. Li, A. Mostafa, N. Abdolrahim, J. Zimmerman, Z. Liang, L. Klinger, J. Yeom, J. Janczak-Rusch, and E. Rabkin, “Solid state dewetting of co-sputtered thin Mo-Cu films accompanied by phase separation”, *TMS Annual Meeting & Exhibition 2025, Las Vegas, NV (Scheduled)*.

S. Qian, A. Mostafa, F. Li, E. Rabkin, and N. Abdolrahim, “Influence of Non-Uniaxial Bending on Twinning and Phase Transformation in Molybdenum Nanowires”, *TMS Annual Meeting & Exhibition 2025, Las Vegas, NV (Scheduled)*.

A. Mostafa, A. Ramasubramaniam, and D. Maroudas, “Thermal conductivity of interlayer-bonded bilayer graphene”, *AIChE Annual Meeting 2023, Orlando, FL*.

A. Mostafa, A. Ramasubramaniam, and D. Maroudas, “Atomistic study of thermal and mechanical properties of graphene-nanodiamond composites”, *MSE Poster Symposium 2023, University of Massachusetts, Amherst*.

M. Chen, A. Mostafa, A. Weerasinghe, A. R. Muniz, A. Ramasubramaniam, and D. Maroudas, “2D diamond superstructures in interlayer-bonded twisted bilayer graphene: Mechanical response and thermal transport from molecular-dynamics simulations”, *AIChE Annual Meeting 2022, Phoenix, AZ*.

M. Chen, A. Weerasinghe, A. R. Muniz, **A. Mostafa**, A. Ramasubramaniam, and D. Maroudas, “Thermomechanical properties of nanodiamond superstructures in interlayer-bonded twisted bilayer graphene”, *AICHE Annual Meeting 2021*, Boston, MA.

**A. Mostafa**, M. Motalab, A. R. Faiyaz, and R. Paul, “Uniaxial and cyclic stress-strain behavior of lead-free solders at the nanoscale”, *AIP Conference Proceedings*, **2019**, Dhaka, Bangladesh.

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## Graduate Thesis

**Afnan Mostafa 2023**, “Thermal conductivity and mechanical properties of interlayer-bonded graphene bilayers”, University of Massachusetts, Amherst, MA, US.

- Addressed two major bottlenecks in graphene-based bilayers (*i.e.*, brittle failure and reduction in thermal conduction)
- Investigated and compared various types of graphene bilayers for thermal management and shear applications
- [MS Thesis DOI: 10.7275/35901268.0](#)

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## Selected Academic Projects

### **FEM formulation in MATLAB and ABAQUS for Hertzian contact**

*Course Instructor: Hesam Askari, Asst. Professor, ME*

*Fall 2023, ME441*

- o Formulated finite element methods from scratch in MATLAB
- o Generated stress and displacement profiles for a Hertzian contact problem
- o Compared such results with ABAQUS-simulated results and theoretical predictions
- o [Report DOI: 10.13140/RG.2.2.32394.48328](#)

### **Machine learning and neural network models across different programming platforms**

*Course Instructor: Brendan Mort, Director, CIRC*

*Fall 2023, DSCC401*

- o Developed machine learning and neural network models for various test cases
- o Compared accuracy among models written in Python and R
- o Analyzed big data using SPARK
- o [GitHub Repository](#)

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## Undergraduate Thesis

**Afnan Mostafa, et al. 2018**, “Uniaxial and cyclic stress-strain behavior of lead-free solders at nanoscale”, Department of ME, Bangladesh University of Engineering and Technology, Dhaka, Bangladesh.

- Investigated cyclic life of environment-friendly lead-free solder materials through atomistic simulations
- Developed atomistic models to predict the lifetime of such solder alloys
- [DOI: 10.1063/5.0037536](#)

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## Skills (\*ordered by decreasing fluency)

<b>Programming*:</b>	Python, Matlab, C/ C++, Bash, SPARK, R, Go, Fortran, MySQL, SPSS, SAS
<b>Simulation Tools*:</b>	LAMMPS, AtomsK, VMD, ANSYS, ABAQUS
<b>Visualization:</b>	Ovito, Vesta, VMD
<b>3D CAD*:</b>	SolidWorks, AutoCAD, OnShape, Adobe Illustrator
<b>Document Preparation:</b>	L <sup>A</sup> T <sub>E</sub> X, MathCAD, Vi, Nano, Microsoft Office Suite
<b>Info-graphic:</b>	Gnuplot, Origin, Plot Digitizer
<b>Job-Scheduling Utility:</b>	Slurm, PBS
<b>Build-Automation:</b>	Make
<b>Others:</b>	Git, High-performance computing, Cluster computing

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## References

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Professor, Mechanical and Industrial Engineering,  
Adjunct, Chemical Engineering,  
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**Dimitrios Maroudas, Ph.D.**

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Affiliated Faculty, Materials Science & Engineering,  
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