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RESEARCH INTERESTS

- Rechargeable batteries: interfacial chemistries of next-generation batteries: metal-S, metal-Se, metal-CO₂
- Electrocatalysis: Nitrogen reduction, CO₂ reduction, and Oxygen/Hydrogen evolution reactions
- Data-driven discovery of materials using Artificial Intelligence (AI) and Machine Learning (ML) techniques
- Understanding graphitization behavior of heavy end aromatic feedstocks

PROFESSIONAL APPOINTMENTS

- **Assistant Professor** 08/2019 - Present
Department of Mechanical Engineering, Wayne State University, Detroit MI - 48202
- **Postdoctoral Research** 09/2016 – 07/2019
Advisor: Prof. Alejandro Strachan
School of Materials Engineering, Purdue University, W Lafayette, IN - 47907
- **Research Intern, RxFF Consulting, LLC** 06/2015 - 08/2015
State College, PA
- **Research Intern, ExxonMobil Research and Engineering** 05/2014 - 08/2014
Corporate Strategic Research, Clinton, NJ
- **Lecturer**, Department of Mechanical Engineering 04/2009 - 08/2011
Bangladesh University of Engineering and Technology, Dhaka, Bangladesh

EDUCATION

- **Ph.D. in Mechanical Engineering** 09/2016
Department of Mechanical and Nuclear Engineering, CGPA: 3.92/4.00
The Pennsylvania State University, University Park, PA-16802
Advisor: Prof. Adri C T van Duin
- **Bachelor of Science in Mechanical Engineering, Salutatorian** 03/2009
Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh CGPA: 3.89/4.00

TEACHING

Graduate level

ME 5995: Materials for Energy Storage and Conversion Fall 2023

Undergrad level

ME 4210: Heat Transfer Theory and Laboratory Fall 2019 - Winter 2023, Winter 2024

ME 2420: Elementary Mechanics of Materials Winter 2021

ME 2500: Numerical Methods using MATLAB Winter 2023

AWARDS

1. **NSF CAREER Award** (2025)
2. Doctoral New Investigator (DNI) award from American Chemical Society, 2021
3. 2021 Ralph E. Powe Junior Faculty Enhancement Award by Oak Ridge Associated Universities (ORAU)
4. 2026 Research Excellence Award from Wayne State University College of Engineering
5. Wayne State 2026 Honorific Award

RESEARCH GRANTS

1. Project: **CAREER: Computational Insights into Interfacial Chemistries in Nonaqueous Batteries**
 - PI: Mahbubul Islam
 - Funding Agency: **National Science Foundation** (Award #2441420)

- Duration: 5 years (03/2025 - 02/2030)
 - Award amount: \$ 540,025
 - https://www.nsf.gov/awardsearch/showAward?AWD_ID=2441420&HistoricalAwards=false
2. Project: **Collaborative Research: An Integrated Experimental and Computational Approach to Reveal Adsorption-Catalysis Cathode Design Principles for Na-S Batteries**
 - PI: Mahbub Islam
 - Funding Agency: **National Science Foundation** (Award #2400109)
 - Duration: 3 years (08/2024-07/2027)
 - Award amount: \$ 285,492
 - https://www.nsf.gov/awardsearch/showAward?AWD_ID=2400109&HistoricalAwards=false
 3. Project: **Elucidating Molecular-level Understanding of Graphitizability of Heavy End Aromatic Feedstocks**
 - PI: Mahbub Islam
 - Funding Agency: **American Chemical Society – Petroleum Research Fund**, (PRF# 65174-DNI6)
 - Duration: 2 years (08/2022-07/2025, no-cost extension)
 - Award amount: \$ 110,000
 - <https://www.acs.org/content/dam/acsorg/funding/grants/prf/about/2021-grants-listing.pdf>
 4. Project: **Rational Design of Electrocatalytically Active Cathode Materials for Lithium-Selenium Batteries**
 - PI: Mahbub Islam
 - Funding Agency: **Ralph E. Powe Junior Faculty Enhancement Awards by Oak Ridge Associated Universities (ORAU)**
 - Duration: 2 years (05/2021-05/2022)
 - Award amount: \$ 10,000
 - <https://tinyurl.com/3svm6w4y>

BOOK CHAPTERS

1. **M M Islam**, M Cherukara, E Antillon, A Strachan “*Shock-induced chemistry: molecular dynamics and coarse grain modeling*” in Computational Approaches to Understanding Chemical Reactivity Under High Pressures, Springer, 2019

PEER REVIEWED JOURNALS

Total published papers: 75

Total Citations: 5550 (as of May 18, 2026, [Google Scholar](#)); h-index 34, i10 index 59.

Notation: *:Directing/corresponding author, †: my student at Wayne State; IF: Impact Factor

2026

1. Pritom R, **Islam MM***. Generative AI-Driven Discovery of Next-Generation Electrolytes for Alkali Metal Batteries. *J. Chem. Inf. Model.* 2026, 66, 7, 3747–3758 [IF: 5.30]
2. Aral, G., **Islam, M. M.**, and Amodeo, J. Molecular dynamics study on the coupled effects of size and pre-existing oxide layer on the compressive mechanical properties of copper nanowires. **Computational Materials Science**, 2026, 262, 114341. [IF: 3.30]
3. [Na-CO₂ Batteries] Jayan, R; Mani, S; **Islam MM***, Mechanistic Insights into CO₂ Capture and Electrochemical Conversion in Nonaqueous Na-CO₂ Batteries, **Journal of Materials Chemistry A**, 2026, 14, 9619-9628

2025

4. [Li-Se Batteries] Pritom, R[†], Nandi, I, Nahian[†], M S, Jayan, R[†], Mojumder, S and **Islam M M*** Computational Discovery of a Novel Double Transition Metal Nitride MXene and its Applications as an Anchoring and Catalytic Material in Li-Se batteries, **Journal of Materials Chemistry A** (2025) <https://doi.org/10.1039/D5TA03099D> [IF: 9.50, Citations: 0]

5. Mani, S; **Islam, MM**,* Tuning Polysulfide Adsorption and Catalytic Activity via Surface Functionalization of Nb₂TiN₂ MXene in Na–S Batteries, **Nanoscale** (2025), 17, 24196–24207, <https://doi.org/10.1039/D5NR03030G> [IF: 5.1]
6. Aral G, **Islam MM**, and Amodeo J, Molecular Dynamics Study on the Coupled Effects of Size and Pre-Existing Oxide Layer on the Compressive Mechanical Properties of Copper Nanowires, **Computational Materials Science** (2025), 262, 114341 [IF: 3.30]
7. Rash, D. van Maarseveen, JH; Geenevasen, JAJ; Tegelaar, E; Pureveen, J; Nijenhuis, RK; Westerveld, N; **Islam, MM**; van Duin, ACT; Stefan Schouten; Sinninghe Damsté, Jaap S. Towards stable chemical fossils for anaerobic ammonium-oxidizing bacteria in palaeoenvironmental studies: novel cyclic aliphatic hydrocarbons as potential dia- and catagenetic products of ladderane lipids, **Geochimica et Cosmochimica Acta** (2025)

2024

8. [Nanomaterials] M.A.S.R. Saadi, F.H. Likhi, M. D. Nath, R. Jayan,[†] F. Zahin, M. S. H. Thakur, Y. Yuan, **M. M. Islam**, R. Panat, A. Karim, P. M. Ajayan, M. M. Rahman, Algae-derived Nacre-like Dielectric Bionanocomposite with High Loading Hexagonal Boron Nitride for Green Electronics. **ACS Nano**, 2024, 18, 48, 33081–33096 [IF: 16.0, Citations: 0]
<https://doi.org/10.1021/acsnano.4c09365>
9. [Graphitization] Nahian,[†] M. S., Pritom, R.,[†] and **Islam, M. M.*** Mechanistic Insights into the Evolution of Graphitic Carbon from Sulfur Containing Polar Aromatic Feedstock, **ACS Applied Materials and Interfaces**, 2024, 16, 41, 55478–55489 [IF: 8.20, Citations: 1]
<https://doi.org/10.1021/acsami.4c12324>
10. [Water Electrolysis] Nagappan, S., Jayan, R.,[†] Rajagopal, N., Krishnan, A.V., **Islam, M.M.*** and Kundu, S., Tailoring Mott–Schottky RuO₂/MgFe-LDH Heterojunctions in Electrospun Microfibers: A Bifunctional Electrocatalyst for Water Electrolysis. **Small**, 2024, p.2403908. [IF: 13.0, Citations: 9]
<https://doi.org/10.1002/sml.202403908>
11. [Mg-CO₂ Batteries] Pritom, R.,[†] Jayan, R.,[†] **Islam, M. M.*** Unraveling the Effect of Single Atom Catalysts on the Charging Behavior of Nonaqueous Mg–CO₂ Batteries: A Combined Density Functional Theory and Machine Learning Approach. **Journal of Materials Chemistry A** 2023, 2335–2348. [IF: 9.50, Citations: 9]
<https://doi.org/10.1039/D3TA06742D>

2023

12. [Mg-CO₂ Batteries] Jayan, R.,[†] **Islam, M. M.*** Advancing Next-Generation Nonaqueous Mg–CO₂ Batteries: Insights into Reaction Mechanisms and Catalyst Design. **Journal of Materials Chemistry A** 2023, 15915–15923. [IF: 9.50, Citations: 5]
<https://pubs.rsc.org/en/content/articlelanding/2023/ta/d3ta03287f/unauth>
13. [Mg-CO₂ Batteries] Jayan, R.,[†] **Islam, M. M.*** Understanding Catalytic Mechanisms and Cathode Interface Kinetics in Nonaqueous Mg–CO₂ Batteries. **ACS Applied Materials and Interfaces** 2023, 15 (39), 45895–45904. [IF: 8.20, Citations: 5]
<https://pubs.acs.org/doi/abs/10.1021/acsami.3c09599>
14. [Graphitization] Nahian, M. S.,[†] Pritom, R.,[†] **Islam, M. M.*** Revealing Mechanistic Insights into Amorphous Graphite Formation from Oxygenated Polar Heavy-End Aromatic Feedstock. **Journal of Physical Chemistry C** 2023, 127 (40), 20146–20156. [IF: 3.20, Citations: 5]
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.3c04899>
15. [OER] Karmakar, A.; Jayan, R.,[†] Das, A.; Kallolorkal, A.; **Islam, M. M.***; Kundu, S. Regulating Surface Charge by Embedding Ru Nanoparticles over 2D Hydroxides toward Water Oxidation. **ACS Applied Materials and Interfaces** 2023, 15 (22), 26928–26938. [IF: 8.20, Citations: 44]
<https://pubs.acs.org/doi/abs/10.1021/acsami.3c05512>
16. [Energetic Materials] Pritom, R.,[†] Nahian, M. S.,[†] Jayan, R.,[†] **Islam, M. M.*** Mechanistic Elucidation of Shock Response of Bis(1,2,4-Oxadiazole)Bis(Methylene) Dinitrate (BOM): A ReaxFF Molecular Dynamics Investigation. **Journal of Applied Physics** 2023, 133 (8), 085101. [IF: 2.70, Citations: 1]
<https://doi.org/10.1063/5.0124675>
17. [Energetic Materials] Hamilton, B. W.; Yoo, P.; Sakano, M. N.; **Islam, M. M.**; Strachan, A. High-Pressure and Temperature Neural Network Reactive Force Field for Energetic Materials. **Journal of Chemical Physics** 2023, 158 (14), 144117. [IF: 3.60, Citations: 21]
<https://pubs.aip.org/aip/jcp/article/158/14/144117/2877981>

18. [Nanomaterials] Aral, G.; *Islam, M. M.* Effect of Oxidation on Mechanical Properties of Copper Nanowire: A ReaxFF (Reactive Force Field) Molecular Dynamics Study. **Journal of Applied Physics** **2023**, 133 (9), 095302. [IF: 2.70, Citations: 2]
<https://doi.org/10.1063/5.0137394>
 19. [OER] Karmakar, A.; Krishnan, A. V.; Jayan, R.;[†] Madhu, R.; *Islam, M. M.**; Kundu, S. Structural Modulation of Low-Valent Iron in LDH-Derived Ni₃Se₄ Nanosheets: A Breakthrough Electrocatalyst for the Overall Water Splitting Reaction. **J. Mater. Chem. A**, **2023**, 11, 10684–10698. [IF: 9.50, Citations: 48]
<https://pubs.rsc.org/en/content/articlelanding/2001/jr/d3ta00868a/unauth>
- 2022
20. [Machine Learning] Malakar, P.; Thakur, M. S. H.; Nahid, S. M.; *Islam, M. M.** Data-Driven Machine Learning to Predict Mechanical Properties of Monolayer Transition-Metal Dichalcogenides for Applications in Flexible Electronics. **ACS Applied Nano Materials** **2022**, 5 (11), 16489–16499. [IF: 5.30, Citations: 31]
<https://pubs.acs.org/doi/abs/10.1021/acsanm.2c03564>
 21. [OER] Madhu, R.; Jayan, R.;[†] Karmakar, A.; Selvasundarasekar, S. S.; Kumaravel, S.; Bera, K.; Nagappan, S.; N Dhandapani, H.; *Islam, M. M.**; Kundu, S. Rationally Constructing Chalcogenide–Hydroxide Heterostructures with Amendment of Electronic Structure for Overall Water-Splitting Reaction. **ACS Sustainable Chemistry and Engineering** **2022**, 10 (34), 11299–11309. [IF: 7.10, Citations: 45]
<https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.2c03292>
 22. [Zn-air batteries] Nair, A. N.; Sanad, M. F.; Jayan, R.;[†] Gutierrez, G.; Ge, Y.; *Islam, M. M.**; Hernandez-Viezas, J. A.; Zade, V.; Tripathi, S.; Shutthanandan, V.; et al. Lewis Acid Site Assisted Bifunctional Activity of Tin Doped Gallium Oxide and Its Application in Rechargeable Zn-Air Batteries. **Small** **2022**, 18 (34), 2202648. [IF: 13.0, Citations: 17]
<https://onlinelibrary.wiley.com/doi/abs/10.1002/smll.202202648>
 23. [Li-S Batteries] Jayan, R.;[†] Nahian, M. S.;[†] *Islam, M. M.** Homogeneous Organometallic Catalysts for Improved Electrochemical Kinetics of Li–S Batteries. **ACS Applied Energy Materials** **2022**, 5 (8), 9782–9790. [IF: 5.50, Citations: 16]
<https://pubs.acs.org/doi/abs/10.1021/acsaem.2c01459>
 24. [Li/Na-S Batteries] Nahian, M. S.;[†] Jayan, R.;[†] *Islam, M. M.** Atomic-Scale Insights into Comparative Mechanisms and Kinetics of Na–S and Li–S Batteries. **ACS Catalysis** **2022**, 12 (13), 7664–7676. [IF: 13.10, Citations: 56]
<https://pubs.acs.org/doi/abs/10.1021/acscatal.2c01174>
 25. [Nanomaterials] Alvi, S. M. A. A.; Faiyad, A.; Munshi, M. A. M.; Motalab, M.; *Islam, M. M.*; Saha, S. Cyclic and Tensile Deformations of Gold–Silver Core Shell Systems Using Newly Parameterized MEAM Potential. **Mechanics of Materials** **2022**, 169, 104304. [IF: 3.40, Citations: 11]
<https://doi.org/10.1016/j.mechmat.2022.104304>
 26. [Li-S Batteries] Mahankali, K.; Gottumukkala, S. V.; Masurkar, N.; Thangavel, N. K.; Jayan, R.;[†] Sawas, A.; Nagarajan, S.; *Islam, M. M.*; Arava, L. M. R. Unveiling the Electrocatalytic Activity of 1T'-MoSe₂ on Lithium-Polysulfide Conversion Reactions. **ACS Applied Materials and Interfaces** **2022**, 14 (21), 24486–24496. [IF: 8.20, Citations: 17]
<https://pubs.acs.org/doi/abs/10.1021/acsaami.2c05508>
 27. [Nanomaterials] Jamil, Md. F.; Jony, Md. S. A. M.; Akash, T. S.; Subad, R. A. S. I.; *Islam, M. M.** Atomistic Elucidation of Mechanical Properties and Fracture Phenomenon of Defective Indium Selenide Monolayer. **Computational Condensed Matter** **2022**, 30, e00637. [IF: 2.60, Citations: 6]
<https://doi.org/10.1016/j.cocom.2021.e00637>
 28. [Na-S Batteries] Nahian, M. S.; Jayan, R.;[†] Kaewmaraya, T.; Hussain, T.; *Islam, M. M.** Elucidating Synergistic Mechanisms of Adsorption and Electrocatalysis of Polysulfides on Double-Transition Metal MXenes for Na–S Batteries. **ACS Applied Materials and Interfaces** **2022**, 14 (8), 10298–10307. [IF: 8.20, Citations: 40]
<https://doi.org/10.1021/acsaami.1c22511>
 29. [MXenes] Jayan, R.;[†] Vashisth, A.; *Islam, M. M.** First-Principles Investigation of Elastic and Electronic Properties of Double Transition Metal Carbide MXenes. **Journal of American Ceramics Society** **2022**, 105 (6), 4400–4413. [IF: 3.90, Citations: 15]
<https://doi.org/10.1111/jace.18394>

30. [Resistive RAM] Urquiza, M. L.; *Islam, M. M.*; van Duin, A. C. T.; Cartoixa, X.; Strachan, A. Atomistic Insights on the Full Operation Cycle of a HfO₂-Based Resistive Random Access Memory Cell from Molecular Dynamics. *ACS Nano* **2021**, 15 (8), 12945–12954. [IF: 16.0, Citations: 39]
<https://doi.org/10.1021/acsnano.1c01466>
31. [Na-S Batteries] Jayan, R.;[†] *Islam, M. M.** Mechanistic Insights into Interactions of Polysulfides at VS₂ Interfaces in Na–S Batteries: A DFT Study. *ACS Applied Materials and Interfaces* **2021**, 13 (30), 35848–35855. [IF: 8.20, Citations: 52]
<https://doi.org/10.1021/acsami.1c10868>
32. [eReaxFF] Leven, I.; Hao, H.; Tan, S.; Guan, X.; Penrod, K. A.; Akbarian, D.; Evangelisti, B.; Hossain, M. J.; *Islam, M. M.*; Koski, J. P.; et al. Recent Advances for Improving the Accuracy, Transferability, and Efficiency of Reactive Force Fields. *Journal of Chemical Theory Computation* **2021**, 17 (6), 3237–3251. [IF: 5.70, Citations: 75]
<https://doi.org/10.1021/acs.jctc.1c00118>
33. [Nanomaterials] Rahman, Md. H.; Chowdhury, E. H.; Bin Shahadat, M. R.; *Islam, M. M.** Engineered Defects to Modulate the Phonon Thermal Conductivity of Silicene: A Nonequilibrium Molecular Dynamics Study. *Computational Material Science* **2021**, 191, 110338. [IF: 3.10, Citations: 31]
<https://doi.org/10.1016/j.commatsci.2021.110338>
34. [Na-S Batteries] Jayan, R.;[†] *Islam, M. M.** Single-Atom Catalysts for Improved Cathode Performance in Na–S Batteries: A Density Functional Theory (DFT) Study. *Journal of Physical Chemistry C* **2021**, 125 (8), 4458–4467. [IF: 3.20, Citations: 70]
<https://doi.org/10.1021/acs.jpcc.1c00467>
35. [Energetic Materials] Ford, J.; Seritan, S.; Zhu, X.; Sakano, M. N.; *Islam, M. M.*; Strachan, A.; Martínez, T. J. Nitromethane Decomposition via Automated Reaction Discovery and an Ab Initio Corrected Kinetic Model. *Journal of Physical Chemistry A* **2021**. [IF: 2.80, Citations: 31]
<https://doi.org/10.1021/acs.jpca.0c09168>
36. [Energetic Materials] Yoo, P.; Sakano, M.; Desai, S.; *Islam, M. M.**; Liao, P.; Strachan, A. Neural Network Reactive Force Field for C, H, N, and O Systems. *Npj Computational Materials* **2021**, 7 (1), 1–10. [IF: 9.70, Citations: 79]
<https://doi.org/10.1038/s41524-020-00484-3>
37. [Li-Batteries] Thangavel, N. K.; Mundhe, S.; *Islam, M. M.*; Newaz, G.; Arava, L. M. R. Probing of Internal Short Circuit in Lithium-Ion Pouch Cells by Electrochemical Impedance Spectroscopy under Mechanical Abusive Conditions. *Journal of Electrochemical Society* **2021**, 167 (16), 160553. [IF: 3.20, Citations: 19]
<https://iopscience.iop.org/article/10.1149/1945-7111/abd452/meta>
38. [Nanomaterials] Akash, T. S.; Subad, R. A. S. I.; Bose, P.; *Islam, M. M.** Nanomechanics of Antimonene Allotropes Under Tensile Loading. *Physical Chemistry Chemical Physics* **2021**, 23, 6241–6251 [IF: 2.90, Citations: 9]
<https://doi.org/10.1039/D0CP05563H>
39. [Nanomaterials] Chowdhury, E. H.; Rahman, Md. H.; Fatema, S.; *Islam, M. M.** Investigation of the Mechanical Properties and Fracture Mechanisms of Graphene/WS₂ Vertical Heterostructure: A Molecular Dynamics Study. *Computational Material Science* **2021**, 188, 110231. [IF: 3.10, Citations: 42]
<https://doi.org/10.1016/j.commatsci.2020.110231>
40. [Nanomaterials] Chowdhury, E. H.; Rahman, Md. H.; Jayan, R.; *Islam, M. M.** Atomistic Investigation on the Mechanical Properties and Failure Behavior of Zinc-Blende Cadmium Selenide (CdSe) Nanowire. *Computational Material Science* **2021**, 186, 110001. [IF: 3.10, Citations: 26]
<https://doi.org/10.1016/j.commatsci.2020.110001>
41. [Nanomaterials] Faiyad, A.; Munshi, M. M. A.; *Islam, M. M.*; Saha, S. Deformation Mechanisms of Inconel-718 at the Nanoscale by Molecular Dynamics. *Physical Chemistry Chemical Physics* **2021**, 23 (17), 10650–10661. [IF: 2.70, Citations: 18]
<https://doi.org/10.1039/D0CP06614A>
42. [Nanomaterials] Oishi, T. M. T.; Malakar, P.; Islam, M.; *Islam, M. M.** Atomic-Scale Perspective of Mechanical Properties and Fracture Mechanisms of Graphene/WS₂/Graphene Heterostructure. *Computational Condensed Matter* **2021**, 29, e00612. [IF: 2.60, Citations: 8]
<https://doi.org/10.1016/j.cocom.2021.e00612>
43. [Nanomaterials] Rahman, M. H.; Islam, M. S.; Chowdhury, E. H.; Bose, P.; Jayan, R.;[†] *Islam, M. M.** Phonon Thermal Conductivity of the Stanene/hBN van Der Waals Heterostructure. *Physical Chemistry Chemical Physics* **2021**, 23 (18), 11028–11038. [IF: 2.70, Citations: 18]
<https://doi.org/10.1039/D1CP00343G>

44. [Nanomaterials] Aral, G.; **Islam, M. M.*** Atomic-Scale Investigation of the Effect of Surface Carbon Coatings on the Oxidation and Mechanical Properties of Iron Nanowires. **New Journal of Chemistry** 2021, 45 (46), 21763–21774. [IF: 2.70, Citations: 1]
<https://doi.org/10.1039/D1NJ05108C>
45. [Na-S Batteries] Jayan, R.;[†] **Islam, M. M.*** Design Principles of Bifunctional Electrocatalysts for Engineered Interfaces in Na–S Batteries. **ACS Catalysis** 2021, 15149–15161. [IF: 13.10, Citations: 39]
<https://doi.org/10.1021/acscatal.1c04739>

2020

46. [Li-S Batteries] Jayan, R.;[†] **Islam, M. M.*** First-Principles Investigation of the Anchoring Behavior of Pristine and Defect-Engineered Tungsten Disulfide for Lithium–Sulfur Batteries. **Journal of Physical Chemistry C** 2020, 124 (50), 27323–27332. [IF: 3.20, Citations: 36]
<https://doi.org/10.1021/acs.jpcc.0c08170>
47. [Energetic Materials] Sakano, M. N.; Hamed, A.; Kober, E. M.; Grilli, N.; Hamilton, B. W.; **Islam, M. M.**; Koslowski, M.; Strachan, A. Unsupervised Learning-Based Multiscale Model of Thermochemistry in 1,3,5-Trinitro-1,3,5-Triazinane (RDX). **Journal of Physical Chemistry A** 2020, 124 (44), 9141–9155. [IF: 2.80, Citations: 58]
<https://doi.org/10.1021/acs.jpca.0c07320>
48. [Nanomaterials] Islam, M.; Thakur, M. S. H.; Mojumder, S.; Al Amin, A.; **Islam, M. M.*** Mechanical and Vibrational Characteristics of Functionally Graded Cu–Ni Nanowire: A Molecular Dynamics Study. **Composite Part B Engineering** 2020, 198, 108212. [IF: 12.70, Citations: 56]
<https://doi.org/10.1016/j.compositesb.2020.108212>
49. [Nanomaterials] Subad, R. A. S. I.; Akash, T. S.; Bose, P.; **Islam, M. M.*** Engineered Defects to Modulate Fracture Strength of Single Layer MoS₂: An Atomistic Study. **Physica B Condensed Matter** 2020, 592, 412219. [IF: 2.80, Citations: 34]
<https://doi.org/10.1016/j.physb.2020.412219>
50. [Energetic Materials] **Islam, M. M.**; Strachan, A. Role of Dynamical Compressive and Shear Loading on Hotspot Criticality in RDX via Reactive Molecular Dynamics. **Journal of Applied Physics** 2020, 128 (6), 065101. [IF: 2.70, Citations: 26]
<https://doi.org/10.1063/5.0014461>
51. [Nanomaterials] Chowdhury, E. H.; Rahman, M. H.; Bose, P.; Jayan, R.; **Islam, M. M.*** Atomic-Scale Analysis of the Physical Strength and Phonon Transport Mechanisms of Monolayer β -Bismuthene. **Physical Chemistry Chemical Physics** 2020, 22 (48), 28238–28255. [IF: 2.90, Citations: 24]
<https://doi.org/10.1039/D0CP04785F>
52. [MXenes/Li-Se Batteries] Jayan, R.;[†] **Islam, M. M.*** Functionalized MXenes as Effective Polyselenide Immobilizers for Lithium–Selenium Batteries: A Density Functional Theory (DFT) Study. **Nanoscale** 2020, 12 (26), 14087–14095. [IF: 5.10, Citations: 51]
<https://doi.org/10.1039/D0NR02296A>
53. [Nanomaterials] Rahman, Md. H.; Chowdhury, E. H.; **Islam, M. M.*** Understanding Mechanical Properties and Failure Mechanism of Germanium-Silicon Alloy at Nanoscale. **Journal of Nanoparticle Research** 2020, 22 (11), 311. [IF: 2.10, Citations: 25]
<https://doi.org/10.1007/s11051-020-05040-0>

2019

54. [Energetic Materials] Hamilton, B. W.; Kroonblawd, M. P.; **Islam, M. M.**; Strachan, A. Sensitivity of the Shock Initiation Threshold of 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB) to Nuclear Quantum Effects. **Journal of Physical Chemistry C** 2019, 123 (36), 21969–21981. [IF: 3.20, Citations: 45]
<https://doi.org/10.1021/acs.jpcc.9b05409>
55. [Nanomaterials] Aral, G.; **Islam, M. M.**; Wang, Y.-J.; Ogata, S.; van Duin, A. C. T. Atomistic Insights on the Influence of Pre-Oxide Shell Layer and Size on the Compressive Mechanical Properties of Nickel Nanowires. **Journal Applied Physics** 2019, 125 (16), 165102. [IF: 2.70, Citations: 6]
<https://doi.org/10.1063/1.5080640>
56. [Nanomaterials] Tripathi, S.; **Islam, M. M.**; Strachan, A. Phonon Thermal Transport in Encapsulated Copper Hybrids. **Journal of Applied Physics** 2019, 125 (4), 045106. [IF: 2.70, Citations: 4]
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57. [Nanomaterials] Das, S.; Mojumder, S.; Rakib, T.; **Islam, M. M.**; Motalab, M. Atomistic Insights into Mechanical and Thermal Properties of Stanene with Defects. **Physica B Condensed Matter** **2019**, 553, 127–136. [IF: 2.80, Citations: 26]
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58. [Energetic Materials] **Islam, M. M.**; Strachan, A. Reactive Molecular Dynamics Simulations to Investigate the Shock Response of Liquid Nitromethane. **Journal of Physical Chemistry C** **2019**, 123 (4), 2613–2626. [IF: 3.20, Citations: 47]
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61. [Energetic Materials] Sakano, M.; Hamilton, B.; **Islam, M. M.**; Strachan, A. Role of Molecular Disorder on the Reactivity of RDX. **Journal of Physical Chemistry C** **2018**, 122 (47), 27032–27043. [IF: 3.20, Citations: 45]
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62. [Nanomaterials] Nahid, S. M.; Nahian, S.; Motalab, M.; Rakib, T.; Mojumder, S.; **Islam, M. M.*** Tuning the Mechanical Properties of Silicene Nanosheet by Auxiliary Cracks: A Molecular Dynamics Study. **RSC Advance** **2018**, 8 (53), 30354–30365. [IF: 3.90, Citations: 28]
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65. [Nanomaterials] Aral, G.; **Islam, M. M.**; Duin, A. C. T. van. Role of Surface Oxidation on the Size Dependent Mechanical Properties of Nickel Nanowires: A ReaxFF Molecular Dynamics Study. **Physical Chemistry Chemical Physics** **2018**, 20 (1), 284–298. [IF: 2.90, Citations: 26]
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2017

66. [Energetic Materials] **Islam, M. M.**; Strachan, A. Decomposition and Reaction of Polyvinyl Nitrate under Shock and Thermal Loading: A ReaxFF Reactive Molecular Dynamics Study. **Journal of Physical Chemistry C** **2017**, 121 (40), 22452–22464. [IF: 3.20, Citations: 58]
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67. [Nanomaterials] Ambrogio, S.; Magyari-Köpe, B.; Onofrio, N.; **Islam, M. M.**; Duncan, D.; Nishi, Y.; Strachan, A. Modeling Resistive Switching Materials and Devices across Scales. **Journal of Electroceramics** **2017**, 1–22. [IF: 1.70, Citations: 34]
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68. [Nanomaterials] Rakib, T.; Saha, S.; Motalab, M.; Mojumder, S.; **Islam, M. M.** Atomistic Representation of Anomalies in the Failure Behaviour of Nanocrystalline Silicene. **Nature Scientific Report** **2017**, 7 (1), 14629. [IF: 3.80, Citations: 36]
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2016

69. [Li-ion Batteries/eReaxFF] *Islam, M. M.*; van Duin, A. C. T. Reductive Decomposition Reactions of Ethylene Carbonate by Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study. **Journal of Physical Chemistry C** **2016**, 120 (48), 27128–27134. [IF: 3.20, Citations: 103]
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71. [Nanomaterials] *Islam, M. M.*; Zou, C.; van Duin, A. C. T.; Raman, S. Interactions of Hydrogen with the Iron and Iron Carbide Interfaces: A ReaxFF Molecular Dynamics Study. **Physical Chemistry Chemical Physics** **2016**, 18 (2), 761–771. [IF: 2.90, Citations: 85]
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72. [eReaxFF] Senftle, T. P.; Hong, S.; *Islam, M. M.*; Kylasa, S. B.; Zheng, Y.; Shin, Y. K.; Junkermeier, C.; Engel-Herbert, R.; Janik, M. J.; Aktulga, H. M.; et al. The ReaxFF Reactive Force-Field: Development, Applications and Future Directions. **Npj Computational Materials**. **2016**, 2, 15011. [IF: 9.70, Citations: 2195]
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2015

73. [Li-S Batteries] *Islam, M. M.*; Ostadhossein, A.; Borodin, O.; Yeates, A. T.; Tipton, W. W.; Hennig, R. G.; Kumar, N.; Duin, A. C. T. van. ReaxFF Molecular Dynamics Simulations on Lithiated Sulfur Cathode Materials. **Physical Chemistry Chemical Physics** **2015**, 17 (5), 3383–3393. [IF: 2.90, Citations: 199]
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74. [2D Nanomaterials] Mojumder, S.; Amin, A. A.; *Islam, M. M.** Mechanical Properties of Stanene under Uniaxial and Biaxial Loading: A Molecular Dynamics Study. **Journal of Applied Physics** **2015**, 118 (12), 124305. [IF: 2.70, Citations: 76]
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2014

75. [Li-S Batteries] *Islam, M. M.*; Bryantsev, V. S.; Duin, A. C. T. van. ReaxFF Reactive Force Field Simulations on the Influence of Teflon on Electrolyte Decomposition during Li/SWCNT Anode Discharge in Lithium-Sulfur Batteries. **Journal of Electrochemical Society**. **2014**, 161 (8), E3009–E3014. [IF: 3.20, Citations: 128]
<https://doi.org/10.1149/2.005408jes>

2. Manuscript currently submitted

76. Mani, S.; *Islam MM**. *Enhancing Nonaqueous Mg–CO₂ Battery Performance via Single-Atom Catalysts on Nitride MXenes*. **Applied Surface Science**
77. Jayan, R.; Mamtani, S.; Pritom, R.; Mao, Z.; Wang, R.; *Islam, MM** Ru-doped MoSe₂ as a Catalytic Polysulfide Host for Accelerated Sulfur Redox Chemistry in Na-S Batteries **ACS Catalysis**
78. Pritom, R.; *Islam MM**, Development of a ReaxFF Force Field for Na-S Chemistry and Its Application to Chemo-Mechanical Evolution of Sodiater Sulfur **Nanoscale**
79. Oliur, R.; Pritom, R.; *Islam MM**, Computational Insights into Enhanced Hydrogen Evolution Reaction (HER) Activity of Nb₂TiN₂ MXenes, **Physical Chemistry Chemical Physics**

CONFERENCE/POSTER PRESENTATION (SELECTED)

1. **Invited Talk**, *M M Islam*, “Computational Insights into Cathode Electrocatalyst Design for Metal-CO₂ Batteries” **248th ECS Meeting**, Chicago, **October 2025**
2. *M M Islam*, “Interfacial Chemistries in Next-Generation Rechargeable Batteries” **243rd ECS Meeting**, Boston, MA, May 2023.
3. **Invited Talk**, *M M Islam*, “*Interfacial Chemistries in Next-Generation Rechargeable Batteries*” **Inorganic Chemistry Seminar Series**, Department of Chemistry, **Wayne State University**, April 2023.
4. **Invited Talk**, *M M Islam*, “*First-principles Elucidation of Interfacial Chemistries in Next-Generation Rechargeable Batteries*” **Paul P. Chevis Endowment Seminar Series**, Chemical Engineering and Materials Science, **Michigan State University**, February 2023.

5. **M M Islam**, R Jayan, Design principles of bifunctional single-atom electrocatalyst for engineered interfaces in Na-S batteries, ACS Fall Meeting, Chicago, August, 2022
6. **M M Islam**, R Jayan, Single-Atom Electrocatalyst for Engineered Cathode Interfaces in Sodium-Sulfur Batteries, 241th ECS Meeting, Vancouver, BC, Canada, May 2022
7. **M M Islam**, **Keynote Speaker**, Energy Storage Discussions, Mexico City, Mexico, October 2019
8. **M M Islam**, B Hamilton, M Sakano, P Yoo, P Liao, A Strachan, "ReaxFF Predictions on Detonation Properties and Reaction Kinetics across the Energetic Materials", *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter*, Portland, OR, June 2019
9. **M M Islam**, A Strachan, "Influence of Combined Normal and Shear Loading on the Hotspot Criticality", *21st Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter, Portland, OR, 2019*
10. Ke Xu, Eli Bostian, A Woepel, H Ding, **M M Islam**, D Guzman, A C Seabaugh, A Strachan, E J Beckman, SF Shirey, "Using Ions to Control Transport in Two-Dimensional Materials for Ion-Controlled Electronics", *2018 IEEE 13th Nanotechnology Materials and Devices Conference (NMDC)*, 2018, Portland, OR
11. **M M Islam**, A Strachan, "On the Determination of Accuracy of Various ReaxFF Models in Predicting Shock-Induced Physics and Chemistry of Energetic Materials", *Gordon Research Conference on Energetic Material*, Newry, ME, June 2018
12. M Sakano, B Hamilton, **M M Islam**, A Strachan, "Role of Molecular Disorder on Reactivity of RDX", *Gordon Research Conference on Energetic Material*, Newry, ME, June 2018
13. **M M Islam**, A Strachan, "Atomistic Insights into Decomposition and Reactions of Energetic Materials under Shock and Thermal Loading" *TMS 2018 Annual Meeting*, Phoenix, AZ, March 2018
14. **M M Islam**, A Strachan, "The Chemistry of Shocked High-energy Materials: Connecting Atomistic Simulations to Experiments", *Bulletin of the American Physical Society*, St. Louis, MO, July 2017
15. M Sakano, B Hamilton, **M M Islam**, A Strachan, "Dependence of hotspot criticality on molecular structure: amorphous vs. crystalline RDX", *Bulletin of the American Physical Society*, St. Louis, MO, July 2017
16. **M M Islam**, A Strachan, "Towards validated chemistry at extreme conditions: reactive MD simulations of shocked Polyvinyl Nitrate (PVN), and Nitromethane" *APS March Meeting*, New Orleans, LA, March 2017
17. **M M Islam**, A Ostadhossein, A C T van Duin, "Carbonaceous Electrode Materials for Lithium-Sulfur Battery Applications: A ReaxFF Reactive Force Field Study", *Carbon Conference*, University Park, PA, July 2016
18. **M M Islam**, G Kolesov, E Kaxiras, A C T van Duin, "ReaxFF reactive molecular dynamics simulations with explicit electrons and applications to battery interfaces"; *AIChE annual meeting*, Salt Lake, UT, November 2015
19. A C T van Duin, **M M Islam**, A Ostadhossein, E Kaxiras, "Applications of the ReaxFF Force Field for Identifying Reactive Properties for Complex Battery Materials and Interfaces", ECS meeting, Phoenix, AZ, October 2015
20. **M M Islam**, G Kolesov, E Kaxiras, A C T van Duin, "Treatment of explicit electrons in the ReaxFF reactive molecular dynamics simulations on battery interfaces"; *250th ACS National Meeting*, Boston, MA, August 2015
21. **M. M Islam**, and S Raman, "Application of reactive molecular dynamics simulations to surfaces and interfaces", *ExxonMobil Research and Engineering summer intern poster*, Clinton, NJ, August 2014
22. M Olguin, **M M Islam**, O Borodin, R Jow, and A C T van Duin, "Molecular dynamics study of oxidation-and reduction-induced solvent decomposition reactions in battery electrolytes", *247th ACS Meeting*, Dallas, TX, 2014
23. **M M Islam**, and A C T van Duin, "Application of the ReaxFF reactive force field in the Li-based rechargeable batteries", *ECS Meeting*, San Francisco, CA, October 2013
24. **M M Islam**, and A C T van Duin, "Application of the ReaxFF reactive force field to study mechanical properties of lithiated sulfur", *12th U.S. National Congress on Computational Mechanics*, Raleigh, NC, July 2013

SIMULATION TOOLKITS

1. M S H Thakur and **M M Islam** (2020), "Thermal Conductivity Simulator," <https://nanohub.org/resources/thermalcond>. (DOI: 10.21981/QXAA-B585).
2. M S H Thakur, M Islam, A A Amin, S Mojumder, **M M Islam** (2019), "LAMMPS Input Structure Generator for Functionally Graded Materials (FGM)," <https://nanohub.org/resources/fgmbuilder>. (DOI: 10.21981/JC41-XT92).
3. S Tripathi, R A Cotter, S Utamsing, **M M Islam**, Mohsen B Kivy, A Strachan (2019), "Random and Special Quasirandom Structure Generator," <https://nanohub.org/resources/sqsatat>. (DOI: 10.21981/0AE8-KB43).

SERVICES

College Level:

- ME Faculty Representative to the Faculty Assembly Executive Committee (FAEC) (AY2023-2025),
- Undergraduate Research Standards Committee (AY2023-2024).

Departmental Level:

- Undergraduate Program Director of Mechanical Engineering Department (03/2024-Present)
- Graduate and Undergraduate Committee (AY2019-2024)
- Faculty search committee (AY2019-2021, 2024, 2025)
- Seminar coordinator (AY2023-2024)
- Marketing Committee (AY2023-2024)

THESIS/DISSERTATION DIRECTED

- **Rahul Jayan, Ph.D.**, Thesis Title: *First-Principles Investigation of Interfacial Chemistries in Room-Temperature Sodium-Sulfur Batteries*, **Summer 2024** (Currently, **Director's Postdoctoral Fellow, Los Alamos National Laboratory (LANL)**).
- **Rahul Jayan**, M.S. Thesis title: *Deciphering cathode catalytic mechanisms and interface kinetics in nonaqueous Mg-CO₂ batteries*, **Fall 2023**.
- **Shahriar Nahian**, M.S. Thesis Title: *Understanding the Graphitizability of heavy-end aromatic feedstocks at the molecular level*. **Summer 2023** (Currently PhD student at Purdue University)

REVIEWER

Journal: (1) Nature, (2) Nature Communications, (3) Nature Catalysis, (4) Journal of Physical Chemistry, (5) Advanced Materials (6) Computational Materials Science, (7) Nature Scientific Reports, (8) ACS Applied Materials and Interfaces, (9) Journal of American Chemical Society, (10) Angewandte Chemie, (11) Carbon, (12) J of Molecular Graphics and Modeling, (13) Theoretical Chemistry Accounts, (14) Journal of Applied Physics (15) Physical Chemistry Chemical Physics (16) Applied Physics Letter (17) Journal of Physical Chemistry Letter, (18) Journal of Chemical Physics, (19) Modelling and Simulation in Materials Science and Engineering (20) Chemical Physics Letter (21) Nanomaterials, (22) Nanoscale, (23) Results in Physics, (24) Canadian Journal of Chemistry, (25) C-Open Access Carbon Research Journal, (26) Energies, (27) Metals, and (28) Fibers, (29) AIP Advances.

Proposal: NSF CBET Panel, NSF CMMT program, American Chemical Society – Petroleum Research Fund.

PREVIOUS AWARDS

- Sustainability Innovation Student Challenge Award (SISCA) proposal writing competition on sustainable energy sponsored by DOW Chemical, 2013. Featured at [Penn State News](#)
- Travel grant from the College of Engineering, Penn State, for attending 224th ECS Meeting, San Francisco, CA
- **Salutatorian**, Department of Mechanical Engineering, BUET, class of 2009
- B.Sc. with **Honors** in Mechanical Engineering, 2009
- Awarded **University Merit Scholarship** for all eight semesters during undergraduate studies
- Awarded **Dean's Scholarship** for all four years of undergraduate studies
- University blazer for leading Bangladesh Robot Team in the ABU ROBOCON 2008 competition

PREVIOUS RESEARCH EXPERIENCE

- Investigated chemical and mechanical and spectroscopic responses of energetic materials such as RDX, HMX, TNT, TATB, CL-20, TEX, Polyvinyl Nitrate, and Nitromethane under shock and thermal loading using ReaxFF reactive MD simulations
- Studied atomistic details of the switching timescales of the electric double layer (EDL) field effect transistors using nonreactive EChemDID simulations
- Developed an explicit electron description of the ReaxFF (*eReaxFF*) method to simulate REDOX reactions. Using eReaxFF method, studied the anode-electrolyte interfacial reduction chemistries of Li-ion batteries
- The eReaxFF code has been incorporated in a leading commercial software in computational chemistry – Amsterdam Density Function (ADF) by SCM Corporation, the Netherlands
- Developed lithium/sulfur ReaxFF force field parameters for simulating the chemo-mechanical properties and failure behavior of lithiated sulfur cathode material

- Studied hydrogen embrittlement, failure behavior, and crack propagation mechanism in iron nanowire using ReaxFF and Embedded Atom Model (EAM) potential
- Designed and fabricated autonomous mobile robots using appropriate technology for ABU Asia-Pacific Robot competition ROBOCON 2007 and 2008 and small-scale industrial applications
- Developed a CFD model for an all-body lifting aircraft to calculate lift to drag ratio for volumetrically equivalent fuselages of different profiles at various flight conditions. Star CCM+ and ANSYS-Fluent were used

LEADERSHIP AND OTHER ACTIVITIES

- **Teaching Assistant**, Department of Mechanical Engineering, Penn State, University Park, PA **08/2011 - 12/2011**
- **Visiting Lecturer**, Department of Mechanical Engineering, AUST, Bangladesh **09/2009 - 06/2011**
- **Visiting Lecturer**, Department of Electrical Engineering, Presidency University, Bangladesh **09/2010 - 06/2011**
- **Team Leader**, Bangladesh Team, 7th Asia-Pacific Robot Contest- **ABU ROBOCON 2008**, India
- **Team Member**, Bangladesh Team, 6th Asia-Pacific Robot Contest- **ABU ROBOCON 2007**, Vietnam