

# Md Mahbulul Islam

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## CURRENT POSITION

### Postdoctoral Research Assistant

School of Materials Engineering  
Purdue University, West Lafayette, IN

09/2016 - Present

Project: Chemistry of high energy materials at extreme conditions of pressure and temperature

## EDUCATION

- **Ph.D. in Mechanical Engineering** 09/2016  
Department of Mechanical and Nuclear Engineering,  
The Pennsylvania State University, University Park, PA-16802  
CGPA: 3.92/4.00  
**Advisor:** Dr. Adri C T van Duin  
**Thesis Title:** Reactive molecular dynamics simulations of lithium secondary batteries: interfaces and electrodes
- **Master of Science in Mechanical Engineering** 06/2011  
Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh  
CGPA: 3.42/4.00
- **Bachelor of Science in Mechanical Engineering, Salutatorian** 03/2009  
Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh  
CGPA: 3.89/4.00

## EXPERTISE IN COMPUTATIONAL CHEMISTRY

- Expertise in physics and chemistry of high-energy materials under shock and thermal loading
- Expert in interfacial chemistry of lithium-ion and lithium-sulfur batteries and electrode material properties
- Developer of a new computational tool for simulating explicit electrons within the framework of ReaxFF reactive force field
- Extensive experience in performing DFT calculations: periodic in VASP, and non-periodic in Jaguar, NWChem, Gaussian
- Expert in ReaxFF force field development for simulating various reactive systems and nanomaterials
- Strong expertise in characterizing material behavior using both reactive and non-reactive molecular dynamics simulations
- Experienced in defects and failure behavior of 2D and bulk materials
- Comprehensive experience in scripting for data analysis, and computational tool development

## RESEARCH/PROFESSIONAL EXPERIENCE

### RESEARCH

#### Research Assistant, Department of Mechanical and Nuclear Engineering, Penn State, University Park, PA 01/2012 – 09/2016

- Developed an explicit electron degrees of freedom in the ReaxFF (*eReaxFF*) method to simulate REDOX reactions
- Using *eReaxFF* method, studying electrode-electrolyte interfacial chemistry of Li-ion batteries
- Studied anode-electrolyte interfacial chemistry and effect of electrolyte additives in lithium-sulfur batteries
- Developed lithium/sulfur ReaxFF force field for simulating chemo-mechanical behavior of lithiated sulfur cathode material
- Investigated stereochemistry of various isomeric configurations of ladderane organic molecules
- Studied carbonaceous materials for lithium-sulfur battery electrodes

#### Masters Research, Department of Mechanical Engineering, BUET, Bangladesh 12/2009 - 06/2011

- 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 was used for this investigation.

#### Undergrad Research, Department of Mechanical Engineering, BUET, Bangladesh 10/2007- 03/2009

- Designed and fabricated autonomous mobile robots for ABU Asia-Pacific Robot competition ROBOCON 2008 and small scale industrial applications.

### SUMMER INTERN

#### RxFF Consulting, LLC, State College, PA (project funded by ExxonMobil) 06/2015 - 08/2015

- Studied hydrogen embrittlement mechanism in iron nanowire using ReaxFF and EAM potential
- Conducted failure behavior, and crack propagation study in structural iron

#### ExxonMobil Research and Engineering, Corporate Strategic Research, Clinton, NJ 05/2014 - 08/2014

- Studied hydrogen interactions with bulk iron and precipitator interfaces using the ReaxFF method
- Investigated NO<sub>x</sub> oxidation chemistries, and performed DFT calculations for Pt/Ni/C/H/O force field development

## TEACHING EXPERIENCE

**Teaching Assistant**, Department of Mechanical Engineering, Penn State, University Park, PA **08/2011 - 12/2011**

- Graded undergrad course homework, proctored examinations, led discussion sessions

**Lecturer**, Department of Mechanical Engineering, BUET, Dhaka, Bangladesh **04/2009 - 08/2011**

- Taught several undergrad courses, instructed lab experiments, supervised undergrad student projects, and acted as an academic advisor of a group of undergrad students

## JOURNAL PUBLICATIONS

- **M M Islam**, A Strachan, "Decomposition and Reaction of Polyvinyl Nitrate under Shock and Thermal Loading: A ReaxFF Reactive Molecular Dynamics Study", *Journal of Physical Chemistry C* (2017)
- T Rakib, S Saha, M Motalab, S Mojumder, **M M Islam**, "Atomistic Representation of Anomalies in the Failure Behaviour of Nanocrystalline Silicene", *Nature Scientific Reports* (accepted)
- S Ambrogio, B Magyari-Kope, N Onofrio, **M M Islam**, D Duncan, Y Nishi, and A Strachan, "Modeling resistive switching materials and devices across scales", *J of Electroceramics* (2017)
- **M M Islam**, and A C T van Duin, "Reductive Decomposition Reactions of Ethylene Carbonate via Explicit Electron Transfer from Lithium: An eReaxFF Molecular Dynamics Study", *Journal of Physical Chemistry C* (2016)
- **M M Islam**, G Kolesov, E Kaxiras, and A C T van Duin, "eReaxFF: A pseudo-classical treatment of explicit electrons within reactive force field simulations", *Journal of Chemical Theory and Computation* (2016)
- T P Senftle, S Hong, **M M Islam**, S B Kylasa, Y Zheng, Y K Shin, C Junkermeier, R Engel-Herbert, M J Janik, H M Aktulga, T Verstraelen, A Grama, and A C T van Duin, "The ReaxFF reactive force-field: development, applications, and future directions", *Nature Computational Materials* (2016)
- **M M Islam**, C Zou, A C T van Duin, and Sumathy Raman, "Interaction of hydrogen with iron and iron carbide interfaces: A ReaxFF molecular dynamics study", *Physical Chemistry Chemical Physics* (2016)
- **M M Islam**, A Ostadhossein, O Borodin, T Yeats, W W Tipton, R G Hennig, N Kumar, and A C T van Duin, "ReaxFF molecular dynamics simulations of the lithiated sulfur cathode materials", *Physical Chemistry Chemical Physics* (2015)
- **M M Islam**, V S Bryantsev, and A C T van Duin, "ReaxFF reactive force field simulations on the influence of teflon on electrolyte decomposition during Li/SWCNT anode discharge in lithium-sulfur batteries", *J. of Electrochemical Society* (2014)
- S Mojumder, A A Amin, and **M M Islam**, "Mechanical properties of stanene under uniaxial and biaxial loading: A molecular dynamics study"; *Journal of Applied Physics* (2015)
- L G J van Bree, **M M Islam**, W I C Rijpstra, D Verschuren, A C T van Duin, J.S. Sinnighe Damsté, J W de Leeuw, "Degradation pathways of des-A-arborene/fermene hydrocarbons in East African lake sediments" (ready to submit)

## CONFERENCE/POSTER PRESENTATION (SELECTED)

- **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
- **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
- 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
- **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
- **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
- **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 City, UT, November 2015
- 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
- **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"; *250<sup>th</sup> ACS National Meeting*, Boston, MA, August 2015
- **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
- 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 model battery electrolytes" *247<sup>th</sup> ACS Meeting*, Dallas, TX, March 2014
- **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

- **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 (USNCCM12)*, Raleigh, NC, July 2013

#### REVIEWER

J of Physical Chemistry, Computational Materials Science, Nanomaterials, Fibers, Results in Physics, Energies, Metals, C — Open Access Carbon Research Journal, AIP Advances, Canadian Journal of Chemistry

#### SOFTWARE SKILLS

- **Computational chemistry**: LAMMPS, ADF, VASP, NWChem, Jaguar, Quantum Espresso, Gaussian, CASTEP, Dmol3
- **Computational Fluid Dynamics (CFD)** : ANSYS Fluent, STAR CCM+
- **CAD**: AutoCAD 2D & 3D, Rhinoceros, GAMBIT
- **Programming**: MATLAB, FORTRAN, ANSI C, C# (sharp), Python

#### AWARDS

- Travel grant from the College of Engineering, Penn State, for attending 224<sup>th</sup> ECS Meeting, San Francisco, CA
- **Salutatorian**, Department of Mechanical Engineering, Bangladesh University of Engineering and Technology, 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

#### LEADERSHIP AND OTHER ACTIVITIES

- **Team Leader**, Bangladesh Team, 7<sup>th</sup> Asia-Pacific Robot Contest- **ABU ROBOCON 2008**, India
- **Team Member**, Bangladesh Team, 6<sup>th</sup> Asia-Pacific Robot Contest- **ABU ROBOCON 2007**, Vietnam
- Supervising a group of students from BUET, Bangladesh to conduct research on 2D materials using molecule simulations

#### MEDIA COVERAGE

- Featured at Penn State news for being selected as top five finalist team in the *Dow Chemical* sponsored *Sustainability Innovation Student Challenge Award (SISCA)* proposal writing competition on sustainable energy at Penn State, November 2013