

Md Mahbubul Islam

265 Blue Course Dr., Apt 11C, State College, PA-16803, Cell Phone: +1-814-880-2356

E-mail: mmi122@psu.edu, mahbub.me.buet@gmail.com; Webpage: www.mahbubislam.com

EDUCATION

- **Ph.D. candidate** **August 2011- present**
Department of Mechanical and Nuclear Engineering,
The Pennsylvania State University, University Park, PA-16802
Advisor: **Prof. Adri C. T. van Duin**
CGPA: 3.92/4.00
- **Master of Science in Mechanical Engineering** **June 2011**
Department of Mechanical Engineering,
Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh
- **Bachelor of Science in Mechanical Engineering** **March 2009**
Department of Mechanical Engineering, *Salutatorian*
Bangladesh University of Engineering and Technology (BUET), Dhaka, Bangladesh

RESEARCH EXPERIENCE

Graduate Research Assistant **Jan 2012 – present**
Department of Mechanical and Nuclear Engineering, Penn State, University Park, PA

- Developing an explicit electron description in the ReaxFF classical force field to describe redox chemistry at the electrode-electrolyte interfaces of Li-based rechargeable batteries.
- Investigating anode-electrolyte interfacial chemistry and electrolyte dissociation mechanism of Li-S batteries using ReaxFF reactive molecular dynamics (MD) simulations.
- Developed Li-S ReaxFF potential to describe Li-S interactions and employed this force field for studying reaction mechanism of lithium- sulfur interaction, mechanical and structural properties of lithiated sulfur cathode of Li-S batteries.
- Studied structural and transport properties of carbonate based electrolyte solvent and lithium salt mixture for Li-ion battery application using ReaxFF MD simulations.
- Studied hydrogen interactions with the Iron and Iron Carbide interfaces to investigate various aspects of hydrogen embrittlement.

Summer Intern **June 2015 - August 2015**

Rx_FF Consulting, LLC, State College, PA

- Studied the mechanical properties of Iron nanowire and analysis of hydrogen induced failure behavior.

Summer Intern **May 2014 - August 2014**

ExxonMobil Research and Engineering, Corporate Strategic Research, Clinton, NJ

- Studied the effect of hydrogen interactions with vacancy and precipitators in Iron using ReaxFF

Masters research **Dec 2009- June 2011**

- Developed a computational fluid dynamics (CFD) model for the 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 **Oct 2007- Mar 2009**

- Designed and fabricated autonomous mobile robots for ABU Asia Pacific Robot competition ROBOCON 2007 and 2008 and for small scale industrial applications.

SKILLS IN COMPUTATIONAL CHEMISTRY

- Classical molecular dynamics
- Free energy sampling methods (metadynamics, umbrella sampling)
- Density functional theory calculation (both periodic and non-periodic)

COMPUTATIONAL SKILLS

- Classical molecular dynamics package: LAMMPS, Amsterdam Density Function (ADF)
- Quantum chemistry: VASP, NWChem, Jaguar, Quantum Espresso, Gaussian, CASTEP, Dmol3
- Programming language: FORTRAN, ANSI C, MATLAB
- Computational fluid dynamics: ANSYS Fluent, STAR CCM+
- Computer aided design: AutoCad 2D & 3D, Rhinoceros, GAMBIT

JOURNAL PUBLICATIONS

5. T. P. Senftle, S. Hong, M M Islam, S. B. Kylasaf, Y. Zheng, Y. K. Shin, C. Junkermeier, R. Engel-Herbert, M. J. Janik, H. M. Aktulga, T. Verstraelen, A. Grama, and Adri C. T. van Duin, "*The ReaxFF Reactive Force-field: Development, Applications, and Future Directions*", npj Computational Materials (accepted)
4. M M Islam, C Zou, Adri 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, DOI: 10.1039/C5CP06108C
3. 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, 118, 124305 (2015)
2. M M Islam, Alireza Ostadhossein, Oleg Borodin, Todd Yeats, W W. Tipton, Richard G. Hennig, Nitin Kumar, and Adri C.T. van Duin, "*ReaxFF Molecular Dynamics Simulations of the Lithiated Sulfur Cathode Materials*", Physical Chemistry Chemical Physics (2015)
1. M M Islam, Vyacheslav S. Bryantsev, and Adri 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. Electrochemical Society (2014)

CONFERENCE/POSTER PRESENTATION

9. Applications of the ReaxFF force field for identifying reactive properties for complex materials and interfaces; Adri van Duin, Chowdhury Ashraf, Abhishek Jain, Alireza Ostadhossein, M M Islam, Yuan Xuan, Oleg Borodin, 2016 TMS Annual Meeting & Exhibition, February 2016, Nashville, TN
8. M M Islam, Grigory Kolesov, Efthimios Kaxiras, Adri 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
7. (Invited) Applications of the Reaxff Force Field for Identifying Reactive Properties for Complex Battery Materials and Interfaces ;Adri CT van Duin, M M Islam, Alireza Ostadhossein, Murali Raju, Sulin Zhang, Efthimios Kaxiras, Oleg Borodin; 228th Electrochemical Society Meeting, Phoenix, AZ, October 2015
6. M M Islam, Grigory Kolesov, Efthimios Kaxiras, Adri 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
5. M. M Islam, and Sumathy Raman, Application of Reactive Molecular Dynamics Simulations to Surfaces and Interfaces, ExxonMobil Research and Engineering summer intern poster, Clinton, NJ, August 2014
4. M M Islam, and Adri C. T. van Duin, *Application of the ReaxFF reactive Force Field in the Li-based rechargeable batteries*, 224 ECS meeting, San Francisco, CA, October 2013
3. M M Islam, Alireza Ostadhossein, and Adri 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
2. Adri van Duin, Murali Raju, M M Islam, *ReaxFF based reactive molecular dynamics simulations on battery interfaces*, ACS National meeting, New Orleans, April 2013
1. Murali Raju, M M Islam, Adri van Duin, Ganesh Panchapakesan, Paul Kent and Andrew Stack , *ReaxFF reactive force field development and applications to reactive interfaces*, Poster presentation, FIRST Center Meeting, Oak Ridge National Lab, Oak Ridge, Tennessee, September 2012

PROFESSIONAL EXPERIENCE

- **Teaching Assistant** **Aug 2011- Dec 2011**
Department of Mechanical and Nuclear Engineering,
The Pennsylvania State University, University Park, PA-16802
Graded course homeworks, proctored examinations, led discussion sessions
- **Lecturer** **April 2009- July 2011**
Department of Mechanical Engineering,
Bangladesh University of Engineering and Technology, Dhaka, Bangladesh
Taught several undergrad courses, instructed lab experiments, supervised group of students on projects, and acted as an academic advisor of group of undergrad students.
- **Adjunct Lecturer** **Nov 2009 - Mar 2011**
Department of Mechanical and Production Engineering
Ahsanullah University of Science and Technology, Dhaka, Bangladesh
Instructed undergraduate lab experiments

AWARDS

- **Salutatorian**, Bangladesh University of Engineering and Technology, 2009
- B.Sc. with **Honors** in Mechanical Engineering
- Awarded **University Merit Scholarship** for all eight semesters during undergraduate studies
- Awarded **Dean's Scholarship** for all four years during undergraduate studies
- **Technical Award** for engineering education at top engineering school in Bangladesh

LEADERSHIP ACTIVITIES

- Selected as top [five finalist](#) team in the Dow Chemical sponsored Sustainability Innovation Student Challenge Award (SISCA) at Penn State for the proposal of "*Li/S Batteries: Converting Environmentally Hazardous Industrial Byproduct Sulfur to High Performance Energy Storage Devices*" November, 2013
- **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.

MEMBERSHIPS

- Student member of American Chemical Society (ACS) and American Institute of Chemical Engineers (AIChE)