Md. Masrul Huda

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Educations

Mississippi State University
Ph.D. in Chemical Enggr. August, 2014-December, 2019
Minor in *Computer Science and Enggr.*
CGPA: 4.00/4.00
Advisor: Neeraj Rai

Bangladesh University of Engineering and Technology
B.Sc. in Chemical Enggr. 2013
CGPA: 3.43/4.00

Skills

Computer Skills: *B: Basic, I: Intermediate, P: Proficient

- **Languages:** C++[P], Fortran[P]
- **Scripting:** Python[P], Bash[P], Awk[P]
- **Parallel Computing:** MPI[P], OpenMP[P], Cuda[I]
- **Data Science:** R[P], PyTorch[I]
- **IDE:** VIM/Black[P]
- **Software Management**: CMake[P], Make[P], GIT[I], PIP[I]
- **Numerical analysis:** Matlab[P], Mathematica[B]
- **OS:** Linux/Unix/*x[P], macOS[P], Windows[I]
- **3D Modeling:** Blender-Python[I]
- **Cheminformatics:** RDKit[I]

Theoretical Skills:
• Molecular dynamics • Monte Carlo • Machine learning • Quantum mechanics • Chemical and Petroleum enggr.

Simulation softwares:
• GROMACS • LAMMPS • CP2K • NAMD • PLUMED • Gaussian • VMD

Computer Science Courses

*For requirement of Minor in CS

- Machine learning
- Computational fundamentals
- Design of parallel algorithms
- Algorithms
- Parallel and distributed scientific computing
- Data science with R

Trainings

International HPC Summer School (IHPCSS) *Ljubljana, Slovenia,* 2016
Training on the key high performance computing (HPC) techniques. 80 participants were selected from European, Canadian, Japanese and U.S. institutions from a competitive application pool.
***Achievement:** 2nd best timing in GPU optimization challenge.

Argonne Training Program On Extreme-Scale Computing (ATPESC) *Argone National Laboratory,* 2016
Comprehensive training to meet exa-scale computing challenges. State of the art techniques of parallel computing were taught by pioneers of HPC domain. A total of 65 participants, consists of graduate students, national lab scientists and post-docs were selected from a highly competitive application pool.

Mira Boot Camp *Argone National Laboratory,* 2015
It trained users of Mira, which was the 6th fastest supercomputer in world ranking during the training period. Performance profiling, software optimization, debugging etc. were covered during boot camp.

Experiences

Mississippi State University
Postdoctoral Associate January, 2020-present
Graduate Research Assistant August, 2014-December, 2019

- Investigating self-assembly of molecular/polymeric gels using molecular dynamics.
- Investigating dye-semiconductor interactions in dye sensitized solar cells (DSSCs) using density functiona theory.
- Studying diffusion of carbohydrates into zeolite nano-structures using molecular dynamics.
- Employing machine learning techniques for discovering optoelectronic materials.
- Developing Monte Carlo molecular simulation suite for high performance computing.
- Automating assignment of force-field parameters to complex polymer using subgraph isomorphism.

- Developing software toolkits to automate simulation task flows. Developed tools are frequently used by fellow graduate students.
- Managing scientific softwares in high performance computing environments. Solid expertise at building/compiling complex scientific softwares from source code in Linux/Unix environment.
- Providing technical supports to fellow graduate students of research group.

PUBLICATIONS

Google Scholar Profile: Md Masrul Huda

Journals **Authors with equal contributions*

1. SM Hashemnejad*, **MM Huda***, N Rai, S Kundu, Molecular insights into gelation of Di-Fmoc-l-Lysine in organic solvent–water mixtures, ACS Omega 2(5), 1864-1874.
2. Zhongxin Chen, Wenqiang Li, Md Abdus Sabuj, Yuan Li, Weiya Zhu, Miao Zeng, Chandra S Sarap, **MM Huda**, Xianfeng Qiao, Xiaobin Peng, Dongge Ma, Yuguang Ma, Neeraj Rai, Fei Huang, Evolution of the Electronic Structure in Open-Shell Donor-Acceptor Organic Semiconductors, Nature communications 12 (1), 1-10
3. SS Venkatesan, **MM Huda**, N Rai, Molecular insights into ionic liquid/aqueous interface of phosphonium based phase-separable ionic liquids, AIP Advances 9 (4), 045115
4. Md Shamim Howlader, SS Venkatesan, H. Goel, **MM Huda**, William T. French, N Rai, Solubility of CO_2 in triglycerides using Monte Carlo simulations, Fluid Phase Equilibria (476), 39-47
5. **MM Huda** and N Rai, Probing Early-Stage Aggregation of Low Molecular Weight Gelator in an Organic Solvent, The Journal of Physical Chemistry B, 124(11), 2277-2288.
6. Md Abdus Sabuj, **MM Huda**, and N Rai, Donor-acceptor conjugated macrocycles with polyradical character and global aromaticity, iScience 23 (11), 101675
7. **MM Huda***, Nusrat Jahan*, and N Rai, Effect of Water Models on Structure and Dynamics of Lignin in Solution, AIP Advances 11 (6), 065024. **Featured, Editor's Pick and Scilight coverage.**
8. Md Abdus Sabuj, **MM Huda**, and N Rai, Benzobisthiadiazole-based high-spin donor-acceptor conjugated polymers with localized spin distribution, Materials Advances 2 (9), 2943-2955. **Popular Advances, and Journal Cover**
9. **MM Huda**, Chinmoy Saha, Nusrat Jahan, WN Wilson and N Rai, Insights into Sorption and Molecular Transport of Aqueous Glucose into Zeolite Nanopores, The Journal of Physical Chemistry B 126 (6), 1352-1364.
10. Nusrat Jahan, **MM Huda**, Quyen Tran, and N Rai, Effect of Solvent Quality on Structure and Dynamics of Lignin in Solution, The Journal of Physical Chemistry B 126 (31), 5752-5764.
11. ZW Windom, Mayukh Dattaa,**MM Huda**, Md Abdus Sabuj, and N Rai, Understanding Speciation and Solvation of Glyphosate from First Principles Simulation, Journal of Molecular Liquids 365, 120154
12. Md Abdus Sabuj, Obinna Muoh, **MM Huda**, and N Rai, Non-Aufbau orbital ordering and spin density modulation in high-spin donor—acceptor conjugated polymers. Physical Chemistry Chemical Physics 24 (38), 23699-23711.
13. Md Abdus Sabuj, **MM Huda**, Chinmoy Saha, and N Rai, Indacenodinaphthothiophene isomers with polyradical character. *(Under review in ACS Omega)*

Conference presentations

1. **MM Huda** and Neeraj Rai, Molecular Dynamics Study of self-assembly of Low Molecular Mass Organic Gelators, AIChE annual meeting 2015, Salt Lake City, UT
2. **MM Huda** and Neeraj Rai, Molecular insights into early stage aggregation of di-Fmoc-L-lysine in binary mixture of organic solvent and water, APS March Meeting, 2017, New Orleans, LA

Conference posters

1. **MM Huda** and Neeraj Rai, Probing the early stage of aggregation of low molecular weight gelator (12-hydroxyoctadecanamide) in organic solvents, 2019, ACS San Diego, CA.
2. **MM Huda** and Neeraj Rai, Probing binding modes of dye molecules on semiconductor surface and their dynamics, 2019, ACS San Diego, CA.

Mentorship

Mentees:

- **Rhet O. Hailey**, Freshman, Mississippi State University
- **Dalton Moran**, Biomedical Engineering, Mississippi State University, 2018 (Software Engr. at HBM Prenscia)
- **Amber Jackson**, Senior, Chemical Engineering, Mississippi State University
- **Mayukh Dutta**, Junior, Chemical Engineering, Mississippi State University
- **Dylan Teas**, Senior, Chemical Engineering, Mississippi State University

Responsibilities:

- Introducing with Linux terminal, bash commands, VIM editor.
- Teaching python and Fortran.
- Teaching the concepts of molecular simulation.

Synergistic Activities

- **President**, Chemical Engineering Graduate Student Association — June, 2018 - August, 2019
- **President**, Bangladesh Association of Mississippi State University — May, 2017 - July, 2018
- **Treasurer**, Bangladesh Association of Mississippi State University — May, 2015 - July, 2016