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], OpenACC[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]

Theoretical Skills:

- Molecular dynamics
- Monte Carlo
- Machine learning
- Quantum mechanics
- Chemical and Petroleum enggr.

Simulation softwares:

- GROMACS
- LAMMPS
- CP2K
- NAMD
- PLUMED
- Gaussian
- VMD

CS Courses

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

Experiences

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

- Investigating self-assembly of molecular/polymeric gels.
- Investigating dye-semiconductor interactions in dye sensitized solar cells (DSSCs).
- Studying diffusion of carbohydrates into zeolite structures.
- Developing Monte Carlo molecular simulation suite for high performance computing.
- Automating assignment of force-field parameters to complex polymer using subgraph isomorphism.
- Developing software tool-kits to automate simulation task flows. Developed tools are frequently used by fellow graduate students of Dr. Rai's research group.
- Managing scientific softwares in high performance computing environments. Solid expertise at building/compiling complex scientific softwares from source code in Linux/Unix environment. For example, I compiled GROMACS (MD simulation package) using Intel package, which was 5X faster and NWChem (Quantum package) was 30X faster than versions managed by system admin of HPC2 at Mississippi State University.
- Providing technical supports to fellow graduate students of research group.

KAFCO (Karnaphuli Fertilizer Company Limited)
Graduate Trainee Engineer April, 2014- June, 2014

- Field visiting of operational units
- Monitoring distributed control system.

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.

Publications

Journals **Authors with equal contributions*

- **MM Huda***, Nusrat Jahan*, and N Rai, Effect of Water Models on Structure and Dynamics of Lignin in Solution, (accepted in AIP advance, **Editor's picks and Scilight coverage**)
- **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.
- 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. (**Editor's recommended**)
- Md Howlader, S. 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
- 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
- Abdus Sabuj, **MM Huda**, and N Rai, Donor-acceptor conjugated macrocycles with polyradical character and global aromaticity, iScience 23 (11), 101675
- 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. (**Selected as backcover**)
- Zhongxin chen , Wenqiang Li , Md Abdus Sabuj , Weiya Zhu , Miao Zeng , Chandra Sekhar, **MM Huda** , Xianfeng Qiao , Xuhui Zhu , Xiaobin Peng , Dongge Ma , Prof. Yuguang Ma , Prof. Junbiao Peng , Neeraj Rai , Fei Huang, Evolution of the Electronic Structure in Open-Shell Donor-Acceptor Organic Semiconductors, (under review in Nature communication)
- **MM Huda**, Chinmoy Saha and N Rai, Probing transport properties of beta-glucose into the zeolite framework (to be submitted).
- **MM Huda**, Chinmoy Saha and N Rai, Understanding the gelation of Di-Fmoc-l-Lysine in binary mixture of water-DMSO, A molecular dynamics study. (in preparation)

Conference presentations

- **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
- **MM Huda** and Neeraj Rai, Molecular Insights into the Gelation of Di-Fmoc-l-Lysine in Organic Solvent–Water Mixtures, APS March Meeting, 2017, New Orleans, LA

Conference posters

- **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.
- **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

Awards

- Travel grants for attending AIChE, APS and ACS conferences.
- Travel grants from Department of Energy to participate ATPESC, Argonne National Laboratory.
- Travel grant from NSF and Bagle College of Engineering, MSU to participate ISSHPCC, Slovenia.
- Government scholarship during the high school.
- Several private scholarships for securing 1st place in high school.
- Scholarship for securing 4th during first term of undergraduate.

Refereneces

Dr. Neeraj Rai
Ergon, Inc. Distinguished Professor and Associate Professor
Dave C Swalm School of Chemical Engineering
Mississippi State University
Email: neerajrai@che.msstate.edu

Dr. Christopher Archibald
Assistant Professor
Department of Computer Science and Engineering
Brigham Young University
Email: archibald@cs.byu.edu