Mirza Galib
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Education:

- PhD, University of Alberta, Canada, 2014
  Department: Chemistry
  Research Area: Theoretical and Computational Chemistry
  Supervisor: Gabriel Hanna
- M.S., University of Dhaka, Bangladesh, 2007
  Department: Applied Chemistry and Chemical Technology
- B.Sc., University of Dhaka, Bangladesh, 2005
  Department: Applied Chemistry and Chemical Technology

Work Experiences:

- Assistant Professor (2022- present)
  - Department of Chemistry, Howard University, Washington DC
- Post Doctorate Research Associate (2021 - 2022)
  - Department of Mechanical Engineering, University of Louisville, KY
  - Supervisor: Badri Narayanan
- Post Doctorate Research Associate (2018 - 2020)
  - Department of Chemistry, University of California, Berkeley
  - Supervisor: David Limmer
- Post Doctorate Research Associate (2015-2017)
  - Chemical Physic group, Pacific Northwest National Lab, Richland, WA, USA
  - Supervisor: Chris Mundy

Summary of Research Interest:

I develop and use computational tools for molecular simulations based on machine learning, quantum mechanics and statistical mechanics to understand material properties at a molecular level. Specific areas of current interest include understanding concentrated electrolytes and solid-electrolyte interfaces relevant to basic energy science, condensed phase materials relevant to neuromorphic computing, and air-water interface relevant to atmospheric chemistry.

Invited Talks:

1. Invited talk at the Department of Physics at Howard University on “Developing machine learning force field to study the reactive uptake of N_2O_5 in the atmospheric aerosol”, Nov, 2022.

2. Invited talk at the group meeting of Cohen group, Department of Chemistry at UC Berkeley on “Elucidating the mechanisms of the reactive uptake of N_2O_5 in the atmospheric aerosol”, May, 2021.
3. Invited talk Invited talk at the group meeting of Head-Gordon group, Department of Chemistry at UC Berkeley on “Developing machine learning tools for the atomistic study of interfacial reactions”, March, 2021.
4. Invited talk at the VCTC (Virtual Conference on Theoretical Chemistry), 2020 on, "Elucidating the mechanisms of the reactive uptake of N_2O_5 in the atmospheric aerosol", July, 2020.
5. Invited talk at the Year 7 annual meeting of CAICE (The center for aerosol impact on chemistry of the environment) on "Molecular dynamics simulations of N_2O_5 hydrolysis", UC San Diego, CA, 2019.
6. Departmental Seminar at Nanyung Technological University on "Ab initio modeling of complex chemical phenomenon in condensed phase", Singapore, May, 2018.
7. Invited talk at the 1st Northwest Pacific Theoretical Chemistry Conference on "Using density functional theory to understand the properties of water”, Richland, WA, USA, 2017.
8. Physical sciences division seminar at PNNL on "Fluctuation phenomena and structure of revPBE water at ambient and high pressure (up to 360 MPa)", Richland, WA, USA, 2016.
9. Invited talk at the 8th Annual Symposium on Theoretical and Experimental Spectroscopy and Dynamics on “The role of hydrogen bonding in the decomposition of H_2CO_3 in water: Mechanistic insights from ab initio metadynamics studies of aqueous clusters”, Jasper, AB, Canada, 2014.
10. Invited talk at the 8th Annual Symposium on Theoretical and Experimental Spectroscopy and Dynamics on “Dissociation and decomposition of carbonic acid in bulk water: An ab-initio metadynamics dynamics study”, Jasper, AB, Canada, August, 2013.

Conference talks/posters:

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1. Poster presentation at Berkeley Statistical Mechanics Meeting on "Understanding reactive uptake of N_2O_5 in atmospheric aerosols via machine learning and AIMD ", UC Berkeley, CA, USA, 2020.
2. Poster presentation at ACS national meeting on "Developing reactive force field from DFT based ab initio molecular dynamics", San Diego, CA, 2019.
3. Poster presentation at the Gordon Research Conference on Liquids on "Understanding reactive uptake of N_2O_5 in atmospheric aerosols via machine learning and AIMD", , Holderness School, NH, USA, 2019.
4. Poster presentation at Berkeley Statistical Mechanics Meeting on "Reactive force field based on DFT and machine learning ", UC Berkeley, CA, USA, 2019.
5. Oral presentation at ACS National Meeting on "Fluctuation phenomena and structure of revPBE water at ambient and high pressure (up to 360 MPa)", San Francisco, USA, 2017.
6. Poster presentation at ACS National Meeting on " First-principles calculations of the K-edge XANES spectra for aqueous Na^+ and for ion pairs of Ca^{2+} with either carbonate or bicarbonate", San Francisco, USA, 2017.
7. Poster presentation at Gordon Research Conference ‘Atomic and Molecular interaction’ on “The role of hydrogen bonding in the decomposition of H_2CO_3 in water: Mechanistic insights from ab initio metadynamics studies of aqueous clusters”, Stonehill College, MA, USA, 2014.

8. Poster presentation at 26th Canadian Symposium on Theoretical and Computational Chemistry on “Mechanistic Insights into the Dissociation and Decomposition of Carbonic Acid in Water Via the Hydroxide Route: An Ab Initio Metadynamics Study”, Concordia University, Quebec, Canada, July, 2014.
9. Poster presentation at 95th Canadian Chemistry Conference and Exhibition on “Mechanistic Insights into the Dissociation and Decomposition of Carbonic Acid in Water Via the Hydroxide Route: An Ab Initio Metadynamics Study”, Calgary, AB, Canada, May, 2012.
10. Oral presentation at 6th Annual Symposium on Theoretical and Experimental Spectroscopy and Dynamics on “Dissociation and decomposition of carbonic acid in water cluster: An ab-initio metadynamics dynamics study”, Jasper, AB, Canada, August 17, 2012.

Publications: (h-index 11, citations 652)

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1. S.Gosh, H. Agarwal, M. Galib et. al., “ Near-Quantitative Predictions of First-Shell Coordination Structure of Hydrated First-Row Transition-Metal Ions Using K-Edge X-ray Absorption Near-Edge Spectroscopy”, ***J. Phys. Chem. Lt.,*** 13,27,6323-6330, 2022.
2. H. Liu, M. Galib et. al. “Controlled Formation of Conduction Channel in Memristive Devices Observed by X-ray Multimodal Imaging”, ***Advanced Materials***, 34(35), 2203209, 2022.
3. K. Bajaj, S. Andres, D. Hofsommer, M. Galib et. al., “Linkage Isomers of a Bis(alkylthiocarbamato)Copper Complex with Antiproliferation Activity”, ***Inorg. Chem.***, 61, 20, 7715-7719, 2022.
4. V.W.D. Cruzeiro, M. Galib, D. T. Limmer, A. W. Goetz, “Uptake of N_2O_5 by aqueous aerosol unveiled using chemically accurate many-body potentials” ***Nature Communications,*** 13, 1266, 2022.
5. S. P. Niblett, M. Galib, and D. T. Limmer, D.T., “Learning intermolecular forces at liquid-vapor interfaces”, ***J. Chem. Phys.***, 155, 164101, 2021. ***[Editor's pick]***
6. M. Galib and D. Limmer, "Reactive uptake of N_2O_5 by atmospheric aerosol is dominated by interfacial process", ***Science***, 371.6532: 921-925, 2021.
7. N. Nguyen, M. Galib and A. Nguyen, "Critical Review on Gas Hydrate Formation at Solid Surfaces and in Confined Spaces: Why and How Does Interfacial Regime Matter?", ***Energy & Fuels,*** 34, 6, 6751-6760, 2020.
8. T. Duignan, T., G. K. Schenter, M. Galib, M. D. Baer, J. Wilhelm, J. Hutter et al., "Quantifying the hydration structure of sodium and potassium ions: taking additional steps on Jacob's Ladder." ***Phys. Chem. Chem. Phys.***, 22, 10641-10652, 2020.
9. M. Galib et al., "Unraveling the Spectral Signatures of Solvent Ordering in K-edge XANES of Aqueous Na^{+}", ***J. Chem. Phys.,*** 149(12), 124503, 2018. ***[Editor's pick]***
10. M. Galib et al., "Supersaturated calcium carbonate solutions are classical." ***Science Advances***, 4(1), eaa06283, 2018.
11. S. Roy, S., M. Galib, M., G. K. Schenter, & C. J. Mundy, "On the relation between Marcus theory and ultrafast spectroscopy of solvation kinetics" ***Chem. Phys. Lt.,*** 692, 407-415, 2017. ***[Invited Frontier Article]***
12. M. Galib, T. T. Duignan, G. K. Schenter, C. J. Mundy, “Mass density fluctuations in Quantum and Classical descriptions of liquid water”, ***J. Chem. Phys.,*** 146, 244501, 2017. ***[Featured by the editor, A Scilight “Using density functional theory to understand the properties of water” on this article was published in AIP Scilight]***

13. M. Galib, M. Baer, L.B. Skinner, C. J. Mundy, T. Huthwelker, G. K. Schenter, C.J. Benmore, J. L. Fulton, "Revisiting the hydration structure of aqueous sodium ions (Na^+)", ***J. Chem. Phys.,*** 146, 084504, 2017.
14. N. Nguyen, A. Nguyen, K. Steel, L. Dang, M. Galib, "Interfacial Gas Enrichment at Hydrophobic Surfaces and the Origin of Promotion of Gas Hydrate Formation by Hydrophobic Solid Particles" ***J. Phys. Chem. C,*** 121(7), 3830-3840, 2017.
15. L.B. Skinner, M. Galib, J. L. Fulton, C. J. Mundy, J. B Parise, Van-Thai Pham, G. K. Schenter, C.J. Benmore, "The structure of liquid water up to 360 MPa from x-ray diffraction measurements using a high Q-range and from molecular simulation", ***J. Chem. Phys.,*** 144, 134504, 2016.
16. M Galib and G. Hanna, "Molecular Dynamics Simulations Predict an Accelerated Dissociation of H_2CO_3 at the air-water Interface", ***Phys. Chem. Chem. Phys.,*** 16, 25573-25582, 2014.
17. M. Galib and G. Hanna, "The role of hydrogen bonding in the decomposition of H_2CO_3 in water: Mechanistic insights from ab initio metadynamics studies of aqueous clusters" ***J. Phys. Chem. B,*** 118 (22), 5983-5993, 2014.
18. M. Galib and G. Hanna, "Mechanistic insights into the dissociation and decomposition of carbonic acid in water via the hydroxide route: An ab-initio metadynamics study", ***J. Phys. Chem. B,*** 115 (50), 15024–15035, 2011.
19. S. T. A Islam, M. Z. Alam, M. Ismail, M. Galib, N. Sharif, and M. Saha, "A Statistical Approach to Alkylation of p-Cresol with Cyclopentanol", ***Asian J. Chem.,*** 22 (2), 1245-1250, 2010.
20. M. Galib, M. Z. Alam, D. Saha, M. Ismail, S. T. A Islam, and M. Saha, "Application of Plackett-Burman Design to tert.-Methylcyclohexylation of p-Chorophenol", ***Chem. Technol. Fuel Oils,*** 45 (5), 336-342, 2009.