HEMANTH H.
DEPARTMENT OF CHEMISTRY, UNIVERSITY OF UTAH
Email: hemanth.haridas@utah.edu
Website: https://hemanthharidas.github.io/

RESEARCH TRAINING

- **University of Utah**, Salt Lake City, USA
  Post Doctoral Research Associate
  Advisor: Prof. Aurora E. Clark
  Duration: 19th Jan 2024 - Current
  - ***Project:*** *Understanding nucleation processes in super concentrated aqueous electrolytes and complementary dissolution of their associated minerals*
  - ***Description:*** *Development of a reactive-type FF that can capture the dissolution of alumina and aggregation of aluminate ions at the solid-liquid interface. Work done in collaboration with Pacific Northwest National Laboratory (PNNL) as part of Ion Dynamics in Radioactive Environments and Materials (IDREAM) Energy Frontier Research Center (EFRC)*
  - ***Deliverables:*** *Developed and integrated a custom LAMMPS pair style for our in-house force field, extending its reactive simulation capabilities in large-scale MD studies. Also carried out atomistic investigations of aluminate-poly-oxo anion condensation pathways, uncovering key mechanistic steps governing aggregation condensation reactions.*

- **Schlumberger**, Pune, India
  Student Intern
  Manager: Dr. Richa Sharma
  Duration: 26th June 2023 - 16th November 2023
  - ***Project:*** *Ab-initio calculations on various surfaces on commercial interest, with particular focus on carbon capture*
  - ***Description:*** *Investigation of binding modes and binding energies for components of syn-gas and producer gas [CO,H_2O,N_2,CO_2] with N-containing 2D surfaces.*
  - ***Deliverables:*** *Performed geometry and energy optimizations of target complexes using the Amsterdam Modeling Suite (AMS), followed by regression analysis on multiple variables to identify key structure–property relationships, supporting rational design of advanced materials.*

- **Indian Institute of Technology Gandhinagar**, Gandhinagar, India
  PhD Scholar, Discipline of Chemistry
  Advisor: Dr. Sairam S. Mallajosyula
  Duration: 27th June 2018 - 29th June 2024
  - ***Thesis:*** *Polarizable Simulations of Nucleobase - Graphene Interactions and Electrolyte Effects: Insights into Nano-Bio Interfaces*
  - ***Description:*** *Investigated the influence of molecular polarizability on the interactions between nucleobases with graphene surfaces, with particular focus on the interfaces.*
  - ***Deliverables:*** *Pioneered the first polarizable graphene parameters in the CHARMM Drude force-field and demonstrated their superior fidelity in reproducing experimental dynamics—capturing ssDNA pore-blockage during graphene translocation and extended nucleobase self-assembly—phenomena that previous non-polarizable models could not describe.*

- **Pondicherry University**, Puducherry, India
  Masters Student, Department of Chemistry
  Advisor: Dr. Musiri M. Balakrishnarajan
  Duration: 3rd July 2017 - 5th May 2018
  - ***Thesis:*** *Computational investigations of novel 2D materials with topologically non-trivial characteristics*
  - ***Description:*** *Investigated the ability of s-indacene type motifs to host Dirac cones using plane-wave DFT calculations.*
  - ***Deliverables:*** *Demonstrated that Hg- and Pt-containing motifs can host Dirac cones, with potential applications in electronics.*

EDUCATION

- **Indian Institute of Technology Gandhinagar**, Gandhinagar, India
  Doctor of Philosophy, Discipline of Chemistry
  Duration: 27th June 2018 - 29th June 2024
  - ***Major Coursework:*** *Quantum Chemistry, Statistical Thermodynamics and its Applications in Chemistry, Molecular Spectroscopy and Data Structures and Algorithms-I*
  - ***CPI:*** *8.67*

- **Pondicherry University**, Puducherry, India
  Master of Science (Five-year Integrated Course) in Chemistry, Department of Chemistry
  Duration: 3rd June 2013 - 5th May 2018
  - ***Major Coursework:*** *Quantum Chemistry, Statistical Thermodynamics and Reaction Dynamics, Symmetry and Group Theory in Chemistry and Spectroscopy: Theory and Applications*
  - ***CPI:*** *8.26*

CODING PROJECTS

- **plank.py**: A basic Hatree-Fock code to calculate orbital energies and total energy of the molecule. Heavy lifting is done using OpenMPI and Cython routines. [GitHub Repository]

- **planck**: A rewrite of plank.py codebase in modern C++ with support for symmetry detection and unrestricted calculations. [GitHub Repository]

PUBLICATIONS

- **H., Hemanth** and Mallajosyula*, S.S.; Graphene: From Solid Support for Nucleobase Assisted Self-Assemblies to Functional Material for DNA Sequencing; *J. Phys. Chem. C*, 2024, **8**, 3091 - 3112; https://pubs.acs.org/doi/10.1021/acs.jpcc.3c08041

- **H., Hemanth** and Mallajosyula*, S.S.; Unveiling DNA Translocation in Pristine Graphene Nanopores: Understanding Pore Clogging via Polarizable Simulations; *ACS Appl. Mater. Interfaces*, 2023, **47**, 55095–55108; https://doi.org/10.1021/acsami.3c12262

- **H., Hemanth**, Mewada, R. and Mallajosyula*, S.S.; Capturing Charge and Size Effects of Ions at the Graphene- Electrolyte Interface Using Polarizable Force Field Simulations; *Nanoscale Adv.*, 2023, **5**, 796 - 804; https://doi.org/10.1039/D2NA00733A.

- **H., Hemanth**, Yadav, P.K. and Mallajosyula*, S.S.; Capturing Concentration Induced Aggregation of Nucleobases on Graphene Surface Through Polarizable Forcefield Simulations; *J. Phys. Chem. C*, 2022, **31**, 13122 - 13131; https://pubs.acs.org/doi/10.1021/acs.jpcc.2c02910

- **H., Hemanth** and Mallajosyula*, S.S.; Polarization influences the evolution of nucleobase-graphene interactions; *Nanoscale*, 2021, **13**, 4060 - 4072; https://doi.org/10.1039/D0NR08796C

TEACHING

- Instructor for 7th i-CoMSE Workshop: Molecular Dynamics Summer School 2024 at Boise State University, ID
  Duration: 8th July 2024 - 12th July 2018
  - ***Description:*** *Led a tutorial session for 40 participants on the topic "FF parameterization of a small molecule", where students were guided through the various steps of FF parameterization, using 2-aminocarboxylic acid as a test case.*

- Teaching Assistant for Solid State Chemistry - I at IIT Gandhinagar (Spring Semester - 2021)
  Duration: 8th January 2021 - 6th May 2021
  - ***Description:*** *Assisted the course faculty in running the course for 30 students, by setting question papers and proctoring exams.*

ACHIEVEMENTS

- Certification in Scientific Writing, Offered by Indian Institute of Technology Gandhinagar.
- Certification in Teaching, Offered by Indian Institute of Technology Gandhinagar.

CONFERENCES AND SYMPOSIUMS

- CECAM Virtual Winter School in Computational Chemistry (Single Figure Presentation)
  February 2021
- International Conference on Nano Science and Nano Technology [ICONSAT] (Poster)
  March 2020
- Theoretical Chemistry Symposium [TCS] (Poster)
  March 2019

COMPUTER SKILLS

- **Computational Chemistry packages**
  - ***ab-initio Packages:*** Gaussian, Orca, CP2K
  - ***classical MD Packages:*** NAMD, CHARMM, LAMMPS, OpenMM, Gromacs
- **Programming/Scripting Languages**
  - Python, C/C++, Fortran
- **Typesetting**
  - LaTeX