HEMANTH.H
UNIVERSITY OF UTAH
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EDUCATION AND TRAINING

- **Pondicherry University**, Puducherry, India
  Master of Science (Five year Integrated Course) in Chemistry, Department of Chemistry
  Advisor: Dr. Musiri M. Balakrishnarajan
  Duration: July 2013 - May 2018

RESEARCH TRAINING

- **University of Utah**, Salt Lake City, USA
  Post Doctoral Research Associate
  Supervisor: Prof. Aurora E. Clark
  Duration: Jan 2024 - Current
  - ***Project:*** *Understanding nucleation processes in super concentrated aqueous electrolytes and complementary dissolution of their associated minerals*
- **Schlumberger**, Pune, India
  Internship Student
  Manager: Dr. Richa Sharma
  Duration: June 2023 - November 2023
  - ***Project:*** *ab-initio calculations on various surfaces on commercial interest, with particular focus on carbon capture*
- **Indian Institute of Technology Gandhinagar**, Gandhinagar, India
  PhD Student, Discipline of Chemistry
  Advisor: Dr. Sairam S. Mallajosyula
  Duration: July 2018 - November 2023
  - ***Thesis:*** *Polarizable Simulations of Nucleobase - Graphene Interactions and Electrolyte Effects: Insights into Nano - Bio Interfaces*

PUBLICATIONS

- **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
- **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**, 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** 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** 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

CODING PROJECTS

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

TEACHING

- Teaching Assistant for Solid State Chemistry - I (Spring Semester - 2021, 31 students).

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 (SFP)
  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**
  - Gaussian, ORCA, NAMD, Gromacs, Quantum Espresso, CHARMM
- **Programming/Scripting Languages**
  - Python, C/C++, Fortran
- **Typesetting**
  - LaTeX

LANGUAGE SKILLS

Malayalam (Native), English (Fluent), Hindi (Fluent), Deutsch (Basic), Spanish (Basic)