Devargya Chakraborty

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Summary

Ph.D. in Chemical Engineering, IIT Patna | B.Tech in Chemical Engineering, HIT

I am a highly motivated professional with a Ph.D. in Chemical Engineering, specializing in Molecular Dynamics Simulation, from the esteemed Indian Institute of Technology, Patna. During my doctoral research, I demonstrated an in-depth understanding of molecular behaviors and interactions using advanced computational techniques. My academic journey began with a Bachelor's degree in Chemical Engineering from the Haldia Institute of Technology, where I consistently displayed a strong academic record with a GPA of 8.75. This laid the foundation for my passion in the field of chemical engineering.

Education

Chemical Engineering (PhD)

Indian Institute of Technology, Patna • Patna, Bihar 01/2025

- Did my PhD in MD simulation, exploring the Interfacial Behavior of Ionic Liquids and DES at diverse substrates.
- Received SERB International Travel grant.
- Won **1st prize** in Oral presentation at ICSPT-2023 held in IIT-Patna.
- Graduated with a GPA of **8.7**

Chemical Engineering (B.Tech)

Haldia Institute of Technology, Haldia • Haldia, West Bengal 07/2019

- Knowledge in different Chemical Engineering Processes (Mass Transfer, Heat Transfer, Fluid Mechanics, Thermodynamics)
- Did my Research Internship from **CSIR-Madurai** Industrial Internship from **IOCL.**
- Graduated with a CGPA of **8.72.**
- Won the Best Oral presentation in **Schemcon-2017** at NIT-Rourkela.

Higher Secondary

Kendriya Vidyalaya No.1 Kalaikunda • Kalaikunda, Kharagpur 04/2015

- Graduated with **92%**

Experience

Junior Research Fellow

Indian Institute of Technology, Patna • Patna, Bihar 07/2019 - 01/2020

- Did my Project on the "Wetting Behavior of Ionic Liquids on different surfaces: Using Molecular Dynamics Simulation".
- Learn about different Open Source softwares like LAMMPS, GROMACS, DL-POLY

Publications

1. Wetting Behavior of Aqueous 1-Alkyl-3-Methylimidazolium Tetrafluoroborate {[Cn MIM][BF4](n= 2, 4, 6)} on Graphite Surface.
2. Cylindrical Droplet of Aqueous Ionic Liquids on Smooth and Pillared Graphite Surface: A Molecular Dynamics Study

Projects

- Project funded by SERB on "MD simulation of Ionic liquids on diverse substrates".
- Project funded by NSM and SERB on "Using Aqueous DES for Enhanced Oil Recovery".

Skills

LAMMPS, GROMACS, VMD, Linux, Python, MATLAB, Shell Scripting, Fortran, C++, DL-POLY

Conference/Workshops

1. FUNMOLSIM-2020, 2. ICHEC-2022, 3. CHEMCON-2022, 4. ICHEC-2023

Languages

English, Hindi, Bengali, Spanish; Castilian