
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

Indian Institute of Technology, Patna

Chemical Engineering (PhD) • Patna, Bihar

01/2025

- Did my PhD in MD simulation, exploring the Interfacial Behavior of Ionic Liquids and DES at diverse substrates.
- Graduated with a GPA of 8.7

Haldia Institute of Technology, Haldia

Chemical Engineering (B.Tech) • 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.

Kendriya Vidyalaya No.1 Kalaikunda

Higher Secondary • Kalaikunda, Kharagpur

04/2015

- Graduated with 92%
 - Got selected in "Regional Mathematics Olympiad"
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Experience

Indian Institute of Technology, Patna

Junior Research Fellow and Senior Research Fellow • Patna, Bihar

07/2019 - Present

- Did my Project on the "Wetting Behavior of Ionic Liquids on different surfaces: Using Molecular Dynamics Simulation".
 - Worked on a Project titled "Interfacial and Wetting behaviour of Aqueous Deep Eutectic Solvent on different Substrates for Enhanced Oil Recovery".
 - Learn about different Open Source MD softwares like LAMMPS, GROMACS, DL-POLY.
 - Worked on with different Quantum Packages like VESTA, Gaussian, ORCA, Quantum-Espresso.
 - Worked on different open-source programmes like MD-Analysis, Pizza, ASE etc.
 - Responsible for looking after HPC systems in the department.
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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*".
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Publications

1. Bhattacharjee, Sanchari, **Devargya Chakraborty**, and Sandip Khan. "Wetting behavior of aqueous 1-alkyl-3-methylimidazolium tetrafluoroborate {[Cn MIM][BF₄]}(n= 2, 4, 6)} on graphite surface." *Chemical Engineering Science* 229 (2021): 116078.
 2. **Chakraborty, Devargya**, Sanchari Bhattacharjee, and Sandip Khan. "Cylindrical droplet of aqueous ionic liquids on smooth and pillared graphite surface: A molecular dynamics study." *Chemical Engineering Science* 277 (2023): 118812.
 3. Kumar, Alok, et al. "Wetting Behavior and Interfacial Dynamics of Aqueous Deep Eutectic Solvents on Diverse Substrates through Molecular Dynamics Simulations: Implications for Enhanced Oil Recovery and Sustainable Applications." *AJIR Abstracts* (2024): 18.
 4. Kumar, Alok, Swasti Medha, **Devargya Chakraborty**, Debashis Kundu, and Sandip Khan. "Wetting and interfacial behavior of aqueous Deep eutectic solvents on Graphite, silica and calcite surfaces: Molecular dynamics study." *Chemical Engineering Science* 296 (2024): 120231.
 5. **Chakraborty, Devargya**, Sana Perween, and Sandip Khan. "Binary imidazolium based aqueous ionic liquid droplet on a rough surface: a molecular dynamics study." *Molecular Physics* (2024): e2409248.
 6. Bhattacharjee, Sanchari, **Devargya Chakraborty**, and Sandip Khan. "Wetting and Interfacial Behavior of Imidazolium-Based Ionic Liquids and Water: A Comprehensive Review." *Fluid Phase Equilibria* (2024): 114252.
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Conference/Workshops

1. Attended Workshop "**FunMolSim-2020**" at IIT-Kanpur organized by Department of Chemical Engineering, IIT-Kanpur.
 2. Attended Workshop on "**LAMMPS**" organized by Sandia Laboratories (2021).
 3. Poster Presentation in "**ICHEC-2022**" organized by IIT-Patna.
 4. Oral Presentation in "**CHEMCON-2022**" organized by IICHE at HBTU Kanpur.
 5. Oral Presentation in "**ICSPT-2023**" organized by IIT-Patna.
 6. Oral Presentation in "**9th EuchemS conference (2024)**" organized ICI and sponsored by ACS and RSC.
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Awards

1. Won 1st prize in "**SCHEMCON-2016**" held in Hyderabad.
 2. Won 1st prize in "**SCHEMCON-2017**" held in NIT-Rourkela.
 3. Won 2nd prize in "**INNOVA-2019**" held in JU.
 4. Won 1st prize in "**ICSPT-2023**" held at IIT-Patna.
 5. Selected for "**International Travel Grant**" by ARNF-SERB.
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Languages

English, Hindi, Bengali, Spanish; Castilian