SWARUP BANERJEE

PROFILE

A computational chemist with 8+ years of experience in molecular dynamics (MD) simulation and programming. My work has primarily involved complex liquid systems, including ionic liquids and deep eutectic solvents, as well as separation chemistry. I have specialized in simulating surfactants and am proficient in using GROMACS and DL_POLY software.

CONTACT

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EDUCATION

Ph.D., Chemistry
07/2017 – 06/2022
Indian Institute of Science Education and Research (IISER) Kolkata
Thesis Topic: *Heterogeneity in Ionic Liquids and Deep Eutectic Solvents: A Molecular Dynamics Simulation Approach*

M.S., Chemistry, CGPA – 8.67
07/2014 – 06/2017
Indian Institute of Science Education and Research (IISER) Kolkata
Thesis Topic: *Molecular Level Understanding of Striped Nanoparticle and Water Interaction: A Molecular Dynamics Simulation Investigation*

WORK EXPERIENCE

Postdoctoral Research Associate, Colorado School of Mines(Prof. Samantha Johnson's Group): 11/2024 – Present

Postdoctoral Research Associate, University of Utah (Prof. Aurora Clark's Group)
12/2022 – 10/2024

- Have learned Chemical Graph Theory and wrote a review paper as lead author.
- Successfully Developed several codes for analyzing reverse micelle structure like cluster distribution, composition analysis, shape determination, SASA calculation.
- Performed simulations over different surfactants and have analyzed their size, shape, and their association pattern with the water clusters.
- Discovered the sensitivity of microemulsion structure, depends upon the surfactant hydrogen bond strength.

Graduate Research Assistant, IISER Kolkata (Prof. Pradip K. Ghorai's Group)
07/2017 – 06/2022

- Worked with the complex structural and dynamical properties of liquid systems, notably Ionic Liquids and Deep Eutectic Solvents (DESs), through extensive computer simulations.
- Discovered the formation of microscopic domains in DESs, formed due to the ion-amide interaction and its influence on dynamic heterogeneity.
- Discovered anomalous motions within DES constituents, revealing insights into solution microheterogeneity and supercooling affinity.
- Discovered the effect of molecular chain length of alcohol on the structure and dynamics of ionic liquid.
- Collaborated on a project leading to the discovery of cosolvent polarity dependence of Ionic Liquid binary mixtures.
- Investigated water mediated weakening of inter-ionic interactions in aqueous mixtures of ionic liquids with quantum chemical calculations and MD simulations.

M. S. Research Assistant, IISER Kolkata (Prof. Pradip K. Ghorai's Group)
07/2014 – 06/2017

- Learned MD simulations and Fortran coding.
- Worked in a project which provides the molecular level understanding of striped nanoparticle and water interaction, a key step of drug delivery mechanism.

ADDITIONAL ACCOMPLISHMENT AND INTEREST

- Senior Research Fellows at IISER Kolkata (Aug 2018 – July 2021).
- Junior Research Fellow at IISER Kolkata (Aug 2016 – July 2018).
- Qualified in Graduate Aptitude Test in Engineering, conducted by Ministry of Human Resource Development in Chemistry (2016).
- Qualified UGC-CSIR National Eligibility Test (NET-June, 2016).
- Qualified Integrated Ph.D. fellowship, Department of Chemical Science, IISER Kolkata (2014 – 2017).
- A professional Quizzer and a cinephile.

SKILLS

Transferable: Critical and Analytical thinking; Independent work, Teamwork, and Collaboration; Problem-solving; Creativity, Curiosity, and Innovation; Leadership; Project Management; Scientific Communication (written and oral); Adaptability; Interpersonal Skills; Work Ethic; Attention to Details.

- Well-versed in **PYTHON**, and **FORTRAN** programming languages and **Bash scripting**. Foundation in **Tcl scripting**.
- OS environments: Mac, Linux, Windows.
- Extensively performed molecular dynamics simulation using **GROMACS, DL_POLY** molecular dynamics package.
- Expertise with **PACKMOL, DL_FIELD, ANTECHAMBER** software for making initial configuration and force field for molecular dynamics simulation.
- Proficient with **Gaussview** and **Gaussian**.
- Software for visualization: **VMD** and **Chimera**
- Experienced with **xmgrace**, **gnuplot** and **PYTHON** for plotting
- Handled PYTHON libraries like **MDAnalysis**, **mdtraj** for the post-processing of simulation data
- Different Graph Theory software like **ChemNetworks**, **Igraph**

RESEARCH OUTPUT

- **S. Banerjee**, Leonardo Leite, Yihui Wei, Jackson Elowitt, Aurora Clark, Modern Chemical Graph Theory, *WIREs Computational Molecular Science* 14, e1729 (2024).
- **S. Banerjee**, P.K. Ghorai, D. Maji, and R. Biswas, Difference in "Supercooling" Affinity between (Acetamide+Na/KSCN) Deep Eutectics: Reflections in the Simulated Anomalous Motions of the Constituents and Solution Microheterogeneity Features, *J. Phys. Chem B* 126, 48, 10146-10155 (2022).
- **S. Banerjee**, P.K. Ghorai, S. Das, J. Rajbangshi, and R. Biswas, Heterogeneous Dynamics, Correlated Time and Length Scales in Ionic Deep Eutectics: Anion and Temperature Dependence, *J. Chem. Phys.* 153, 234502 (2020).
- J. Rajbangshi, **S. Banerjee**, P.K. Ghorai, and R. Biswas, Cosolvent polarity dependence of solution structure in [BMIM][PF_6]$^+$ acetonitrile/1, 4-dioxane/hexane binary mixtures: Insights from composition-dependent Voronoi polyhedra analyses, iso-surfaces and radial distribution functions, *J. Mol. Liq.* 317, 113746 (2020).
- S. Konar, A. Sharma, **S. Banerjee**, P.K. Ghorai, and R. Biswas, Water-mediated weakening of inter-ionic interactions in aqueous mixtures of ionic liquid: An investigation combining quantum chemical calculations and molecular dynamics simulations, *Chem. Phys.* 524, 31 (2019).

Manuscript under preparation:

- **S. Banerjee**, J. Elowitt, A. Clark, Exploring Phase Modifier Interactions in Microemulsion , Manuscript in Preparation.
- **S. Banerjee**, P.K. Ghorai, and R. Biswas, Heterogeneous Dynamics, Correlated Time and Length Scales in Ionic Deep Eutectics: Cation and Temperature Dependence, Manuscript to be Submitted.
- **S. Banerjee**, P.K. Ghorai, and R. Biswas, Hydrogen Bond, and Re-Orientation Dynamics, in Ionic Deep Eutectics: Anion and Temperature Dependence, Manuscript to be Submitted.
- **S. Banerjee**, and P.K. Ghorai, Effect of Molecular Chain Length of Alcohol on the Structure and Dynamics of $[HMIM][PF_6]$ Ionic Liquid: A Molecular Dynamics Simulation Approach, Manuscript to be submitted.