Anupama Sharma

Ph.D. Computational Sciences

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Google Scholar

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About Me

I am a Research Associate at IIIT Hyderabad with a PhD in Computational Sciences. My interests span liquids at interfaces, solvation, IDPs, and integrating MD with AI/ML based approaches. I aim to advance computational tools and multiscale modeling to uncover mechanisms in complex chemical and biomolecular systems for advance therapeutics.

Programming Skills

- Fortran
- Bash Scripting
- Python
- tcl/tk
- Awk
- Perl

Scale: 0 (basic skills) - 6 (expert).

Software and Packages

- Operating system : Ubuntu, Windows, macOS
- HPC job scheduling and resource handling via SLURM.
- Gromacs, AMBER, NAMD, CHARMM-GUI, Auto Dock Vina, Schrodinger, Alphafold, Proteinx Server, Gaussian, CP2K, psi4, Mulitwfn
- GaussView, Avogadro, VMD, Pymol, ChemDraw, Chimera, Xmgrace, gnuplot

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Education

2018 - 2025 **Ph.D. Computational Sciences**

Central University of Punjab, Bathinda, Punjab, India

- **Thesis Title** : *Structure and Dynamics of Complex Liquids Inside Confined Environment.*
- **Skills acquired** - Classical MD using GROMACS, NAMD, AMBER and nonequilibrium or Enhanced sampling Methods.
- Statistical Analysis and Force-Field Parameterization.
- IR-Spectra, dynamic, and structural property extraction from simulations.

2016 - 2018 **M.Sc Chemistry (Medicinal Chemistry)**

Central Univeristy of Punjab, Bathinda, Punjab, India

- Thesis Title : In-vitro and In-silico study of essential oil components for *Eucalyptus tereticornis* as antibacterial agents.
- Skills: Bacterial culture preparation and Agar well diffusion assay, MIC (Minimum Inhibitory Concentration) determination, Schrödinger, SwissADME, PyMOL, Discovery Studio.

2016 - 2018 **B.Sc Chemistry (Honours)**

University of Delhi, Shyam Lal College, New Delhi, India

- Graduated with 68.59% (First division)

Online Courses Attended

Oct 2021 to Jul 2022 **Foundations of Modern Machine Learning conducted** by, IIIT Hyderabad.

Work Experience

March 2025 – present **Research Associate I**

R&D, International Institute of Information Technology (IIIT), Hyderabad, India

- **Project Title** : Carbon Allotrope Dispersion in Ionic Liquids using Enhanced Sampling Simulations.

July 2024 – Feb 2025 **Senior Research Fellow**

I-HUB Data Foundation, International Institute of Information Technology (IIIT), Hyderabad, India

- Developing automated workflows in python and tcl/tk for HES simulations, mentoring interns, and analyzing ligand residence times from steered MD simulations. Preparation and correction of final Manuscript.
- **IDP project**, supported students with simulation and analysis tasks and wrote custom analysis and visualization codes in Fortran and Python.
- I worked in **quantum/classical modeling** of the diastereoselective Henry reaction catalyzed by the BmHNL and AtHNL enzyme. My contributions included identifying catalytic triad and simulating active-site interactions, which fed into subsequent DFT studies.

Teaching Experience

- Teaching Assistant, CCNSB, IIIT-Hyderabad
  Course: Biomolecular Structure Interaction and Dynamics (SC3.321), Monsoon-2024
  Course: Physics of Soft Condensed Matter (S25SC2:301), Spring-2025
  Course: General and Structural Chemistry (S25SC2:101), Spring-2025

Achievements

- (CSIR-NET/JRF-2017,Dec) All India Rank in Chemical Sciences - 126
- Graduate Aptitude Test in Engineering (GATE-2018) Gate Score - 331
- Common University Entrance Test (CUCET(Ph.D.))-2018
- Common University Entrance Test (CUCET(Postgraduation))-2016

Workshop & Conferences

- CECAM Conference MD@60-2024 : Poster Presentation on ''Micro-solvation of Propofol in Propylene Glycol-Water Binary Mixture : Molecular Dynamics Simulation Studies.''
- TCB-2022, NIPER-Mohali : Poster Presentation on ''Effect of Confinement On Water Dynamics: Dependence of Temperature and Diameter of Carbon Conduits. ''
- Workshop on ''Introduction to gaussian : Theory and practice, Hyderabad'' (Jan 20-24, 2020)

Referee Details

- Dr Sudip Chakraborty (Asst. Prof.)
  Central Univeristy of Punjab, India
  sudip.chakraborty@cup.edu.in
- Prof. U. Deva Priyakumar (Prof.)
  Centre Head, Center for Computational Natural Sciences and Bioinformatics (CCNSB)
  deva@iiit.ac.in
- Dr. Diwakar Kumar (Assoc. Prof.)
  Assam University, Silchar, India
  diwakar11@gmail.com
- Dr. Rakesh Srivastava (Asst. Prof.)
  Vellore Institute of Technology, Bhopal, India
  rakeshsrivastava@vitbhopal.ac.in

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Research Publications

6. Roy, R.; Gahatraj, I.; **Sharma, A.**; Kumar, V.; Paul, R.; Kumar, D.; Bhattacharya, P.; Borah, A. Potentials of Cepharanthine and Tomatidine as Novel LpxC and TLR4 Inhibitors to Mitigate Gut-Mediated Inflammation in Parkinson's Disease: A High-Throughput Investigation through Molecular Docking and Dynamic Simulation. *Biotech.*,(**2025**), *15(7),1–24.*
5. **Sharma, A.**; Anand, M.; & Chakraborty, S. Influence of CTAB Reverse Micellar Confinement on the Tetrahedral Structure of Liquid Water. *J. Phys. Chem. B.*,(**2025**), *129(4), 1289–1300*.
4. Saha, S.;**Sharma, Anupama**; Bhowmik, D.; & Kumar, D. Investigation into in silico and in vitro approaches for inhibitors targeting MCM10 in Leishmania donovani: a comprehensive study. *Mol. Divers.*, (**2024**),*1-16*.
3. Nandi, R.; **Sharma, A.**; Priya, A.; & Kumar, D. Integrating Traditional QSAR and Read-Across-Based Regression Models for Predicting Potential Anti-Leishmanial Azole Compounds. *Mol. Divers.*, (**2024**), *28,1–25.*
2. Gahatraj, I.; Roy, R.; **Sharma, A.**; Phukan, B. C.; Kumar, S.; Kumar, D.; Pandey, P.; Bhattacharya, P.; Borah, A. Identification of Molecular Interactions of Pesticides with Keratinase for Their Potential to Inhibit Keratin Biodegradation. *In Silico Pharmacol.*,(**2024**),*12(1),54*.
1. **Sharma, A.**; Kumar, V.; Chakraborty, S. Micro-Solvation of Propofol in Propylene Glycol–Water Binary Mixtures: Molecular Dynamics Simulation Studies. *J. Phys. Chem. B.*,(**2023**), *127(51), 11011–11022.*

Featured on the Cover Page of JPCB, Vol.-127(51), (Dec, 28, 2023).

Submitted Work

- PLAS-HES-5k - A dataset of non-native protein-ligand conformations and binding affinities for machine learning applications in drug discovery. ***NeurIPS 2025 Datasets and Benchmarks.***
- Mechanistic Aspects of Carbon Nanotube Dispersion in Imidazolium-based Room Temperature Ionic Liquids. ***PCCP, CP-ART-06-2025-002215***

Collaborative Experience

I have worked with different research groups in collaboration with :

- **Dr. Diwakar:** Contributed to multiple research projects, with a primary focus on molecular dynamics (MD) simulations. Additionally, played a supportive role in applying machine learning techniques to biomolecular systems.
- **Dr. Rakesh:** Led the development of PLAS-HES-5k, a comprehensive dataset comprising non-native protein-ligand conformations and associated binding affinities. This resource is designed to facilitate machine learning applications in drug discovery, particularly in improving the prediction of ligand binding poses and affinities.