Prantar Dutta

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Research Interests

Molecular Simulation, Density Functional Theory, Machine Learning, Cheminformatics, Porous Materials

Education

University of Montpellier *Oct 2024 – present*
PhD in Chemistry

Indian Institute of Technology Kanpur *Jul 2018 – Aug 2020*
MS in Chemical Engineering
GPA: 9.67/10

Jadavpur University *Aug 2014 – May 2018*
BS in Chemical Engineering
GPA: 8.42/10

Academic Experience

French National Centre for Scientific Research (CNRS) *Oct 2024 - present*
Doctoral Researcher, Institute Charles Gerhardt Montpellier *Montpellier, France*

Project: Metal-Organic Frameworks for Hydrogen/Methane Separation | **Advisor:** Guillaume Maurin

- Exploring metal-organic frameworks (MOFs) and their composites using molecular dynamics (MD), Monte Carlo, density functional theory, and machine learning to design adsorbents for hydrogen/methane separation
- Investigating the adsorption and transport mechanisms of gas mixtures in nanoporous materials

Indian Institute of Technology Kanpur *Jan 2019 - Aug 2020*
Graduate Researcher, Computational Nanoscience Lab *Kanpur, India*

Project: Drug-Lipid Interactions in Multicomponent Membranes | **Advisor:** Jayant K Singh

- Modeled structural, thermodynamic, and drug release characteristics of a supramolecular liposome for delivering a proprietary anti-cancer drug using MD simulations (Collaboration with **Akamara Biomedicine**)
- Investigated the effect of polymer conjugation on the structure, phase behavior, and drug interaction characteristics of lipid bilayers using MD simulations and enhanced sampling

Indian Institute of Technology Kanpur *May 2017 - July 2017*
Summer Research Intern, Heterogeneous Catalysis Lab *Kanpur, India*

Project: Reduction Characteristics of Supported Nickel Catalysts | **Advisor:** Goutam Deo

- Studied the effect of process parameters on the reducability of silica-supported nickel oxide using temperature programmed reduction (TPR) setup, modeled the reaction kinetics, and proposed a mechanism

Jadavpur University *Jan 2017 - Nov 2017*
Undergraduate Researcher *Kolkata, India*

Project: Hydrogen Generation from Ammonia Borane | **Advisor:** Kajari Kargupta

- Synthesized, characterized (SEM, XRD, FTIR), and tested high-performance graphene-supported copper-cobalt bimetallic catalysts for hydrolysis of ammonia borane to determine optimum catalyst composition

Professional Experience

TotalEnergies *Oct 2024 - present*
Researcher, CO_2 and Sustainability R&D *Pau, France*

- Collaborating with research and engineering teams (experimental, computational, process design, pilot-scale testing) to develop technologies for hydrogen separation from methane and nitrogen
- Translating molecular-scale insights of material behavior into adsorption process design strategies

Tata Consultancy Services Research *Sep 2020 - Jun 2024*
Researcher, Physical Sciences *Pune, India*

- Synergized molecular simulations and deep learning (DL) to predict the thermodynamic properties and biological activities of small molecules
- Developed DL-based virtual pipelines for high-throughput screening of industrially relevant molecules
- Co-developed data-driven frameworks for classifying and selecting ingredients for formulating cosmetics
- Delivered R&D consulting projects for a British food and beverage company and an Indian paints company to drive digital transformation in product design
- Led cross-functional collaborations between Research, Business, and IT teams and mentored 3 interns

Achievements

- **CIFRE Fellowship** by French National Association for Technical Research (ANRT) for doctoral studies, 2024
- **Academic Excellence Award** by Indian Institute of Technology Kanpur, 2018 and 2019
- **Graduate Aptitude Test in Engineering (GATE) Fellowship** by the Government of India, 2018-2020
- **Students-Undergraduate Research Graduate Excellence (SURGE) Fellowship** by Indian Institute of Technology Kanpur for summer internship, 2017
- **Certificate of Merit** and **Central Sector Scholarship** by the Government of India for outstanding performance in school leaving examination, 2014

Teaching Activities

- **Teaching Assistant, 5-day workshop on *Fundamentals of Molecular Simulations*** (Feb 2020)
  Conducted hands-on tutorial on GROMACS for 50+ participants, including PhD students and postdocs
- **Teaching Assistant, *Introduction to Molecular Simulations*** (Fall 2019)
  Designed and graded programming assignments and final course projects for 10 students

Skills

Programming and Scripting: Python, MATLAB, Bash
Computational Chemistry: GROMACS, LAMMPS, RASPA, VASP, VMD, PLUMED, AutoDock Vina
Data Science and Machine Learning: NumPy, SciPy, Pandas, Scikit-learn, Keras/TensorFlow, PyTorch
Cheminformatics: RDKit, Open Babel, DeepChem

Publications

Journal Articles:

1. **P Dutta**, K Gajula, D Jain, R Gupta, and B Rai, Computational Screening of Umami Tastants using Deep Learning, *Molecular Diversity* (2024)
2. **P Dutta**, D Jain, R Gupta, and B Rai, Classification of tastants: A deep learning based approach, *Molecular Informatics*, **42**, e202300146 (2023)
3. **P Dutta**, D Jain, R Gupta, and B Rai, Deep learning models for the estimation of free energy of permeation of small molecules across lipid membranes, *Digital Discovery*, **2**, 189-201 (2023)
4. **P Dutta**, D Pramanik, and JK Singh, Phase Behavior of Pure PSPC and PEGylated Multicomponent Lipid and Their Interaction with Paclitaxel: An All-Atom MD Study, *Langmuir*, **37**, 10259-10271 (2021)

Book Chapters:

1. **P Dutta**, D Jain, R Gupta, and B Rai, Predictive Machine Learning Models for Olfaction, *Olfactory Receptors: Methods and Protocols* (part of *Methods in Molecular Biology*), Springer (in press)

Patents:

1. Method and System for Estimation of Free Energy of Permeation, Inventors: **P Dutta**, D Jain, R Gupta and B Rai, US Patent App. 18/163,215, EP Patent App. 23153750.7 (2023)