Manajit Das, Ph.D.

Email: manajit@icredd.hokudai.ac.jp
Date of Birth: 01 October 1996
Current Address: Sapporo, Hokkaido, 060-0808, Japan
Phone: +91 9948324905
Website — GitHub — Google Scholar

Research Interests

- Computational Exploration of Reaction Mechanism Networks
- Machine Learning for Chemical Reactivity and Selectivity Prediction
- Generative Models for Reaction and Mechanism Prediction (Transformers, Flow Matching)
- Graph Neural Networks for Molecular and Reaction Modeling
- Cheminformatics and Data-driven Reaction Discovery

Education

Ph.D. in Computational Chemistry, IIT Bombay, India 2019–2026
Thesis: Machine Learning Studies on Yield, Selectivity, and Mechanisms of Organic Reactions
Supervisor: Prof. Raghavan B. Sunoj

M.Sc. in Chemistry, IIT Hyderabad, India (CGPA: 9.8/10) 2017–2019
Graduated with Institute Gold Medal (Highest CGPA) and Silver Medal (Department Topper).
Project: Synthesis and Characterization of Cs_3FeCl_5 and $Cs_2FeP_2S_6$.
Supervisor: Prof. Jai Prakash

B.Sc. in Chemistry, University of North Bengal, India (69.12%) 2014–2017

Research Experience

- Developed ML models for predicting enantioselectivity in asymmetric relay Heck reactions, achieving accurate and generalizable performance.
- Created graph-based deep-learning architectures for reaction-mechanism prediction with improved interpretability over sequence-based models.
- Conducted in-depth reviews on chemical language models and solvation effects in reaction mechanisms.
- Performed DFT calculations including transition-state searches and mechanistic exploration of organic reactions.

Selected Publications

1. **Das, M.***; Sharma, P.*; Sunoj, R. B. Machine Learning Studies on Asymmetric Relay Heck Reaction—Potential Avenues for Reaction Development. *J. Chem. Phys.* **2022**, *156*, 114303.
2. Hoque, A.*; **Das, M.***; Baranwal, M.; Sunoj, R. B. ReactAIvate: A Deep Learning Approach to Predicting Reaction Mechanisms and Unmasking Reactivity Hotspots. *European Conference on Artificial Intelligence* **2024**, *392*, 2645–2652.

3. **Das, M.**; Ghosh, A.; Sunoj, R. B. Advances in Machine Learning with Chemical Language Models in Molecular Property and Reaction Outcome Predictions. *J. Comp. Chem.* **2024**, *30*, 1160–1176.
4. **Das, M.**; Gogoi, A. R.; Sunoj, R. B. Molecular Insights on Solvent Effects in Organic Reactions as Obtained through Computational Chemistry Tools. *J. Org. Chem.* **2022**, *87*, 1630–1640.
5. **Das, M.***; Hoque, A.*; Baranwal, M.; Sunoj, R. B. DeepMech: A Machine Learning Framework for Chemical Reaction Mechanism Prediction. *Chem. Sci.* **2026**

6. Jana, S.; Panigrahi, G.; Narayanswamy, S.; Ishtiyak, M.; **Das, M.**; Bhattacharjee, P. P.; Niranjan, M. K.; Prakash, J. Synthesis, Crystal Structure, Optical Absorption Study, and Electronic Structure of Cs_3FeCl_5. *Solid State Sci.* **2020**, *100*, 106064.

**equal contribution*

Conferences and Presentations

- Poster, Asia Pacific Association of Theoretical and Computational Chemists (APATCC), Vietnam, 2023.
- Poster, 27th European Conference on Artificial Intelligence (ECAI), Spain, 2024.
- Talk, In-house Symposium, Department of Chemistry, IIT Bombay, India, 2024.
- Poster, Prime Minister Research's Fellowship Annual Symposium, IIT Hyderabad, India, 2025.

Skills

Programming Languages: Python, Bash (Shell Scripting)

Machine Learning & Deep Learning: PyTorch, TensorFlow, DGL, Scikit-learn, Transformer Architectures, Pre-training & Fine-tuning of Chemical Language Models, Graph Neural Networks (GNNs), Representation Learning, Hyperparameter Optimization (Optuna)

High Performance Computing (HPC): Linux Cluster Computing, NVIDIA DGX A100, SLURM/PBS Job Scheduling, Multi-GPU Training, CUDA Acceleration, Bash Automation, Conda Environment Management

Computational Chemistry: Gaussian, GaussView, ORCA, Molden, Avogadro

Cheminformatics: RDKit, Open Babel, NetworkX, Molecular Fingerprints, Molecular Descriptors, SMILES/SMARTS Processing, Reaction Templates, Jupyter Notebook, Google Colab

Version Control & Collaboration: Git, GitHub, Branching Strategies, Pull Requests, Code Review, Issue Tracking, LaTeX

Scientific Data Processing & Visualization: NumPy, Pandas, PubChem/ChEMBL/USPTO Dataset Processing, Matplotlib, Seaborn

Awards and Achievements

- Prime Minister's Research Fellowship (PMRF), 2020–2024

- Institute Gold Medal, IIT Hyderabad
- Silver Medal (Department Topper), IIT Hyderabad
- National Eligibility Test, All India Rank 59, Dec 2017
- Certificate of Academic Excellence, IIT Hyderabad

Teaching Experience

Teaching Assistant, IIT Bombay 2020–2021
CH-504 Computational Chemistry; CH-792 Communication Skills; CH-105 Organic and Inorganic Chemistry
Content Creation (Assignments, Projects, Exercises), Conducted Lab Sessions, Grading, Doubt and Crib Sessions.

PMRF Teaching Assistant 2022–2024
Mechanisms in Organic Chemistry (NPTEL Course); Undergraduate Lectures at R.J. College and V.G. Vaze College, Mumbai.