Dibyendu Maity

Ph.D. in Physics (Theoretical) · Computational Biophysics

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Research Profile

My research develops and applies machine-learning-guided methods for sampling and characterising rare events in molecular systems, with emphasis on adaptive and weighted-ensemble sampling strategies for transition-path discovery and pathway-resolved kinetics. I use representation learning and statistical mechanics to construct data-driven collective variables and to map complex free-energy landscapes, and I build open-source scientific software that makes these methods accessible for molecular dynamics and materials-simulation workflows.

Ph.D. thesis submitted, University of Calcutta. Available for postdoctoral research positions from late 2026.

Education

Ph.D. in Physics (Theoretical) 2021--2026
University of Calcutta / S. N. Bose National Centre for Basic Sciences, Kolkata
Thesis Title: *Development and Application of Machine Learning Approaches for Prediction, Identification and Sampling Problems in the Field of Molecular Modeling and Simulation*
Advisor: Prof. Suman Chakrabarty
Thesis submitted

M.Sc. in Physical Sciences 2019--2021
University of Calcutta / S. N. Bose National Centre for Basic Sciences, Kolkata
Marks: 79.80%

B.Sc. in Physics (Honours) 2016--2019
Midnapore College, West Bengal
Marks: 81.25%

Higher Secondary (WBCHSE) 2016
Ananda Nagar Srinath Vidyapith, Anandanagar
Marks: 94.0%

Secondary (WBBSE) 2014
Ananda Nagar Srinath Vidyapith, Anandanagar
Marks: 94.43%

Selected Publications

S. Shahid, **Dibyendu Maity**, Suman Chakrabarty. "CoWERA: A Temporal Coherence Guided Binless Resampling Algorithm for Weighted-Ensemble Based Estimation of Rare-Event Kinetics." *The Journal of Chemical Physics* 2026, *164*, 134111. DOI: 10.1063/5.0320586.

S. Pal, **Dibyendu Maity**, J. Chakraborty, S. Jha, K. Sarma, N. Koner, S. Chakrabarty, D. Das. "Pathway Controlled Phase Separation of Minimal Building Blocks Utilizing a Dissociative Chemical Transformation." *Angewandte Chemie International Edition* 2026, e1914460. DOI: 10.1002/anie.1914460.

S. Sarkar, R. Saha, A. Dutta, R. Chattopadhyay, **Dibyendu Maity**, I. Biswas, A. Mondal, A. Ghosh, R. Ganguly, A. K. Santra, U. Garain, D. Mitra, S. Chakrabarty. "Microwave-Assisted Thermal Profiling of Blood: A Potential Biomarker for Differentiating Cancer and Non-Cancer States." *Journal of Medical Engineering & Technology* 2026, 1–16. DOI: 10.1080/03091902.2026.2698512.

Dibyendu Maity, Shaheerah Shahid, Suman Chakrabarty. "PathGennie: Rapid Generation of Rare Event Pathways via Direction-Guided Adaptive Sampling Using Ultrashort Monitored Trajectories." *Journal of Chemical Theory and Computation* 2025, *21*, 11377–11389. DOI: 10.1021/acs.jctc.5c01244.

Dibyendu Maity, Suman Chakrabarty. "IceCoder: Identification of Ice Phases in Molecular Simulation

Using Variational Autoencoder." *Journal of Chemical Theory and Computation* 2025, *21*, 1916–1928. DOI: 10.1021/acs.jctc.4c01298.

S. K. Bhaumik, **Dibyendu Maity**, I. Basu, S. Chakrabarty, S. Banerjee. "Efficient Light Harvesting in Self-Assembled Organic Luminescent Nanotubes." *Chemical Science* 2023, *14*, 4363–4374. DOI: 10.1039/D3SC00375B.

R. Sahoo, **Dibyendu Maity**, D. S. S. Rao, S. Chakrabarty, C. V. Yelamaggad, S. K. Prasad. "Dimer-Parity-Dependent Odd-Even Effects in Photoinduced Transitions to Cholesteric and TGB Smectic-C* Mesophases: Experiments and Simulations." *Physical Review E* 2022, *106*, 044702. DOI: 10.1103/PhysRevE.106.044702.

Dibyendu Maity, Shaheerah Shahid, S. Bhattacharya, R. Majumdar, Suman Chakrabarty. "Quantitative Pathway-Resolved Kinetics from Neural Network-Guided Weighted Ensemble Simulations." *ChemRxiv* 2026. DOI: 10.26434/chemrxiv.15005553/v1.

Scientific Software

TRAILS-MD (*Python*): Lightweight, engine-agnostic framework for lineage-aware adaptive molecular dynamics sampling.
https://github.com/TeamSuman/Trails-MD

PathGennie (*Python*): Direction-guided adaptive-sampling framework for rapidly generating rare-event transition pathways.
https://github.com/dmighty007/PathGennie

IceCoder (*Python / PyTorch*): Unsupervised representation-learning framework for ice polymorph and liquid environment classification.
https://github.com/dmighty007/IceCoder

SolOrder (*Python / C++*): Local solvation and structural order parameter analysis utilities for molecular simulations.
https://github.com/dmighty007/SolOrder

Conference Presentations & Invited Talks

Poster presentation, Computational and Data-Driven Advanced Materials (CDAM 2026), CSIR–Central Glass and Ceramic Research Institute, Kolkata, India, 7–8 April 2026. **Poster Award**.

Poster presentation and lightning talk, Workshop on Machine Learning, Enhanced Sampling, and Dynamical Surrogate Models for Glassy and Adaptable Materials, University of Chicago Center in Delhi, New Delhi, India, 30 March–1 April 2026.

Poster presentation, Biophysics Today, S. N. Bose National Centre for Basic Sciences, Kolkata, India, 2–4 December 2025.

Poster presentation, Recent Advances in Modeling Rare Events (RARE 2025): Methods and Applications, Khajuraho, Madhya Pradesh, India, 9–12 March 2025.

Invited lecture, Supramolecular Chemistry Discussion 2024, IISER Kolkata, Kolkata, India, 8 December 2024.

Poster presentation and lightning talk, CHEMDOJO 3.0, 1–4 October 2024.

Poster presentation, JNCASR–CECAM Conference: MD@60, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India, 26–29 February 2024. **Best Poster Award**.

Poster presentation, Lightning Talk, and Hackathon, 2nd Discussion Meeting on Machine Learning for Molecular Sciences 2024 (ML4MS2024), Gokulam Grand, Thiruvananthapuram, Kerala, India, 1–4 February 2024.

Poster presentation, "Identification/Classification of Ice Phases in Molecular Simulation using Variational Autoencoder," Theoretical Chemistry Symposium 2023 (TCS-2023), Department of Chemistry, Indian Institute of Technology Madras, Chennai, India, 7–10 December 2023.

Poster presentation, Physical Chemistry Symposium 2023 (SoPhyC-2023), inaugural meeting of the Society of Physical Chemistry, Indian Institute of Technology Kanpur, Kanpur, India, 29–31 October 2023.

Poster presentation, National Conference on Recent Advances in Chemistry: Theoretical and Computational Aspects (RAC-TCA 2022), Department of Chemistry, NIT Meghalaya and North-Eastern Hill University, India, 18–20 November 2022. **Best Poster Award**.

Awards & Recognition

- **INSPIRE Scholarship for Higher Education (SHE)**, Department of Science and Technology, Government of India (2016–2019). Awarded under the Innovation in Science Pursuit for Inspired Research (INSPIRE) programme; eligibility based on being within the top 1% of the WBCHSE board examination.
- **GATE 2021 — Physics**, Graduate Aptitude Test in Engineering (2021). Qualified with All India Rank 177.
- **National Graduate Physics Examination (NGPE)**, Indian Association of Physics Teachers (IAPT) (2019). Recognized among the national top 26 students in NGPE-2019.
- **JEST 2019 — Physics**, Joint Entrance Screening Test, JEST Consortium (2019). Qualified with All India Rank 191.
- **IIT JAM 2019 — Physics**, Joint Admission Test for M.Sc., Indian Institutes of Technology (2019). Qualified with All India Rank 898.

Technical & Computational Expertise

Molecular simulation: Molecular Dynamics, Enhanced Sampling, Metadynamics, Umbrella Sampling, Adaptive Sampling, Rare-Event Sampling, Langevin Dynamics, Weighted Ensemble.

Machine Learning: Representation Learning, Autoencoders, Variational Autoencoders, Deep Learning, data-driven collective variables, pathway analysis.

Programming: Python, NumPy, SciPy, PyTorch, MDAnalysis, MDTraj, C++, Bash.

Simulation / Scientific Software: GROMACS, OpenMM, PLUMED, Git, Linux/HPC clusters.

Last updated August 2026