Bidhan Chandra Garain, Ph.D.

Marie Skłodowska-Curie Postdoctoral Fellow, Department of Chemistry, University College London (United Kingdom)

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Professional Summary

Computational chemist and AI/ML researcher with a Ph.D. in Theoretical Chemistry and postdoctoral experience in **molecular modeling for discovery applications**. Skilled in **deep learning (CNNs, RNNs, ensembles)**, uncertainty quantification, active learning, and cheminformatics workflows. Experienced in **structure-based and ligand-based** approaches, translating complex molecular datasets into actionable insights for **drug discovery and materials development**.

Professional Experience

01/05/2025 – Ongoing

❖ **Marie Skłodowska-Curie Postdoctoral Fellow, Department of Chemistry, University College London (United Kingdom)**

- Designing **active learning pipelines** to couple electronic-structure calculations with ML, reducing computational cost in NAMD workflows.

14/11/2023 – 30/04/2025

❖ **Postdoctoral Researcher, ICR, Aix-Marseille Universite (France)**

- Co-developed **ULaMDyn**: open-source package for unsupervised learning in molecular dynamics (dimensionality reduction + clustering for trajectory data).
- Mapped emissive conformations to uncover **key structural motifs**, providing insight for molecular design and optimization.
- Developed **deep ensemble and evidential ML models** in PyTorch for excited-state and molecular property prediction with post-hoc calibration for reliability.

04/07/2023 – 08/11/2023

❖ **Research Associate, Theoretical Sciences Unit (TSU), JNCASR (India)**

- Built **ensemble ML workflows** for predicting OLED and photophysical properties, integrating cheminformatics descriptors and deep learning.

Education

01/08/2018 – 03/07/2023

❖ **Ph.D. in Theoretical Chemistry**, Theoretical Sciences Unit (TSU), JNCASR (India)
Thesis title: ***Computational Perspectives on Triplet exciton Harvesting: A Combined Ab Initio and Machine Learning Investigation*** Supervisor: Prof. Swapan K Pati (pati@jncasr.ac.in)

08/2016 – 07/2018

❖ **Master's with *Physical Chemistry* Specialization**, Jadavpur University (India)
Thesis title: ***Alkaline hydrolysis of methyl violet: Kinetic and mechanistic studies.***
Supervisor: Prof. Ambikesh Mahapatra Marks Obtained: **82.4 %**

08/2013 – 07/2016

❖ **Bachelor's with *Chemistry* (Major)**, Jadavpur University (India) Marks Obtained: **76.7 %**

Publications

**** as corresponding author***

1. ***MELTS: Fully Automated Active Learning for Fewest-Switches Surface Hopping Dynamics***
   Matheus de Oliveira Bispo, Rafael Souza Mattos, Max Pinheiro Jr, ***Bidhan Chandra Garain***, Pavlo O Dral, Mario Barbatti
   Journal of Chemical Theory and Computation, 21 (22), 11390-11400 (2025).

2. **ULaMDyn: Enhancing Excited-State Dynamics Analysis Through Streamlined Unsupervised Learning**
   Max Pinheiro Jr, Matheus O Bispo, Rafael S Mattos, Mariana Telles do Casal, ***Bidhan Chandra Garain****, Josene M Toldo, Saikat Mukherjee, Mario Barbatti
   Digital Discovery, 4(3), 666-683 (2025).

3. **Conformational Dynamics of the Pyrene Excimer**
   Giovanni Parolin, ***Bidhan Chandra Garain***, Saikat Mukherjee, Giovanni Granucci, Stefano Corni, Mario Barbatti
   Physical Chemistry Chemical Physics, 26(47), 29351-29363 (2024).

4. **Unleashing Ambient Triplet Harvesting Pathways in Arylene Diimides via Modular, Non -Covalent Charge-Transfer Interactions**
   Anju Kongasseri, Swadhin Garain, Shagufi Ansari, ***Bidhan Chandra Garain***, Sopan Wagalgave, Utkarsh Singh, Swapan Pati, Subi George
   Chemistry of Materials, 35(18), 7781-7788 (2023).

5. **Tailoring Dual Emissions from Pyromellitic Diimide Derivatives through Substitution: A Theoretical Perspective**
   Bidhan Chandra Garain, Swapan K. Pati
   Theoretical Chemistry Accounts, 142(8), 70 (2023).

6. **Unraveling the Efficiency of Thioxanthone-Based Triplet Sensitizers: A Detailed Theoretical Study**
   Bidhan Chandra Garain, Swapan K. Pati
   ChemPhysChem, 24(8), e202200753 (2023).

7. **Room Temperature Charge-Transfer Phosphorescence from Organic Donor–Acceptor Co-crystals**
   Swadhin Garain, Shafugi Naz Ansari, Anju Ajayan Kongasseri, ***Bidhan Chandra Garain***, Swapan K. Pati, Subi J. George
   Chemical Sciences, 13(34), 10011-10019 (2022).

8. **Anion–π Induced Room Temperature Phosphorescence from Emissive Charge-Transfer States**
   Swadhin Garain, Sopan M. Wagalgave, Anju Ajayan Kongasseri, ***Bidhan Chandra Garain***, Shagufi Naz Ansari, Gopa Sardar, Dinesh Kabra, Swapan K. Pati, Subi J. George
   Journal of the American Chemical Society, 144(24), 10854–10861 (2022).

9. **Chiral Arylene Diimide Phosphors: Circularly Polarized Ambient Phosphorescence from Bischromophoric Pyromellitic Diimides**
   Swadhin Garain, Souvik Sarkar, ***Bidhan Chandra Garain***, Swapan K. Pati, Subi J. George
   Angewandte Chemie, 134(11), e202115773 (2022).

10. **Delineating Conformation Control in the Photophysical Behaviour of a Molecular Donor–Acceptor–Donor Triad**
    Bidhan Chandra Garain, Shubhajit Das, Swapan K. Pati
    ChemPhysChem, 22(22), 2297-2304 (2021).

11. **Light-Harvesting Supramolecular Phosphors: Highly Efficient Room Temperature Phosphorescence in Solution and Hydrogels**
    Swadhin Garain, ***Bidhan Chandra Garain***, Muthusamy Eswaramoorthy, Swapan K. Pati, Subi J. George
    Angewandte Chemie International Edition, 60(36), 19720-19724 (2021).

12. **Arylene Diimide Phosphors: Aggregation-Modulated Twin Room Temperature Phosphorescence from Pyromellitic Diimides**
    Swadhin Garain, Suman Kuila, ***Bidhan Chandra Garain***, Meenal Kataria, Aditya Borah, Swapan K. Pati, Subi J. George
    Angewandte Chemie International Edition, 60(22), 12323-12327 (2021).

13. **Intersystem Crossing in Boron-Based Donor–Spiro–Acceptor Organic Chromophore: A Detailed Theoretical Study**
    Bidhan Chandra Garain, Pralok K. Samanta, Swapan K. Pati
    The Journal of Physical Chemistry A, 125(31), 6674-6680 (2021).

14. **Ambient Room Temperature Phosphorescence and Thermally Activated Delayed Fluorescence from a Core-Substituted Pyromellitic Diimide Derivative**
    Suman Kuila, Swadhin Garain, Gangadhar Banappanavar, ***Bidhan Chandra Garain***, Dinesh Kabra, Swapan K. Pati, Subi J. George
    The Journal of Physical Chemistry B, 125(17), 4520-4526 (2021).

15. **Nitric Oxide Sensing Through 1,2,3,4-Oxatriazole Formation from Acylhydrazide: A Kinetic Study** Abu Saleh Musha Islam, Rahul Bhowmick, ***Bidhan Chandra Garain***, Atul Katarkar, Mahammad Ali ***The Journal of Organic Chemistry,*** 83(21), 13287-13295 (2018).

Preprints

1. **Uncertainty Calibration in Molecular Machine Learning: Comparing Evidential and Ensemble Approaches**
   Bidhan Chandra Garain*, Max Pinheiro Jr, Matheus O Bispo, Mario Barbatti
   Under Revision ***Chemistry A European Journal***

2. **Improved Prediction of Maximum EQE in TADF-based OLEDs Through Ensemble Learning**
   Bidhan Chandra Garain*, Swapan K Pati

   Chemrxiv 2022

Conference Presentation

Poster Presented Online Poster at ***In-House Symposium***, 2021 held in ***Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore.***

Poster Presented Poster at ***Theoretical Sciences Unit Day***, 2021 held in ***Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore.***

Poster Presented Online Poster at ***International Winter School***, 2021 held in ***Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore.***

Poster Presented Online Poster at ***DAE Symposium on Current Trends in Theoretical Chemistry (CTTC-2020)*** held in ***BARC, Mumbai.***

Poster Presented Online Poster at ***Theoretical Chemistry Symposium (TCS),*** 2021 held in ***IISER Kolkata.***

Talk Presented Talk on "***Intersystem Crossing in Boron-Based Donor-Spiro-Acceptor Organic Chromophore: A Detailed Theoretical Study***" at ***Theoretical Sciences Unit Day***, 2022.

Talk Presented Talk on "***Improved Prediction of Maximum EQE in TADF-based OLEDs Through Ensemble Learning***" at **In-House symposium, JNCASR, 2022**.

Talk Presented Talk on " ***Enhancing Uncertainty Quantification in Chemical Modeling: A Comparative Study of Deep Evidential Regression and Ensembles with Post-Hoc Calibration***" at **AI and Physical Sciences @Aix Marseille University, 2024**.

Grants, Awards and Scholarships

1. ***Marie Skłodowska-Curie Actions (MSCA) postdoctoral fellowship*** under the 2023 call with Rachel Crespo-Otero at University College London (UK).

2. ***Physical Chemistry Chemical Physics (PCCP) Poster Prize*** at **Theoretical Chemistry Symposium (TCS 2021)** IISER Kolkata.

3. ***Joint five years research fellowship and lifetime lectureship award (all India rank 22)*** by **Council of Scientific and Industrial Research (CSIR),** India, 2018.

4. ***All India Rank 103*** in ***Graduate Aptitude Test Engineering (GATE)*** in Chemistry, 2018.

5. ***Five years INSPIRE scholarship*** awarded by **Department of Science and Technology (DST), India**, 2013.

Supervising graduate students

1. I supervised a master's student at JNCASR, **Utkarsh Singh**, whose research already led to a publication in *Chemistry of Materials* titled 'Unleashing Ambient Triplet Harvesting Pathways in Arylene Diimides via Modular, Non-Covalent Charge-Transfer Interactions' (Anju Kongasseri, Swadhin Garain, Shagufi Ansari, Bidhan Chandra Garain [fellow], Sopan Wagalgave, Utkarsh Singh [master's student], Swapan Pati, Subi George, *Chemistry of Materials*, 35(18), 7781-7788, 2023). Additionally, a preprint is currently in preparation. These projects helped Utkarsh in the completion and submission of his master's thesis.

2. At University College London, I am supervising another master's student **Wu Lance** working on Spatiotemporal Clustering of Non-adiabatic dynamics trajectories.

Open-Source Contributions

I have experience contributing to ULaMDyn a Python-based, open-source package designed to automate the unsupervised machine learning analysis of large datasets generated by NAMD simulations. ULaMDyn integrates seamlessly with the Newton-X platform and employs advanced dimensionality reduction and clustering techniques to uncover hidden patterns in molecular trajectories, enabling a more intuitive understanding of excited-state processes.

Other Interests

Online Certifications in Machine Learning and Artificial Intelligence

1. ***Online Course AI SHIKSHA: An Introduction to Machine Learning, 2021.***
   Centre for Development of Advanced Computing (C-DAC), India
2. ***Introduction to Deep Learning, 2021***
   Centre for Development of Advanced Computing (C-DAC), India
3. ***Online Course on Python for Scientific Computing, 2021***
   National Institute of Technology, Warangal (NITW), India
4. ***Online Course on Deep Learning, 2022***
   One-Fouth Labs, India
5. ***IBM Machine Learning Professional Certificate*** through ***COURSERA***
   1. Exploratory Data Analysis for Machine Learning (Done)
   2. Supervised Machine Learning: Regression (Done)
   3. Supervised Machine Learning: Classification (Ongoing)
6. ***Generative Adversarial Networks (GANs) Specialization*** through ***DEEPLEARNING.AI***
   1. Build Basic Generative Adversarial Networks (GANs) (Done)
   2. Build Better Generative Adversarial Networks (GANs) (Ongoing)

Other Skills

Language	***Bengali, English, Hindi***
Coding	***Fortran 77, Fortran 90, and Python***

Software	***Electronic structure codes*** (Gaussian, ADF, ORCA, Turbomole, VASP)
	Quantum Dynamics codes (Multi Configuration Time Dependent Hartree (MCTDH), Qutip), **Newton-X, MELTS**
	Machine Learning and Deep Learning (Pytorch and Scikit-Learn), **ULamDyn**
	Visualization (Matplotlib, Plotly and Seaborn), **Git**