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Professional Experience

14/11/2023 – Ongoing	Postdoctoral Researcher, ICR, Aix-Marseille Universite (France) Supervisor: Prof. Mario Barbatti (mario.barbatti@univ-amu.fr)
04/07/2023 – 08/11/2023	Research Associate, Theoretical Sciences Unit (TSU), JNCASR (India) Supervisor: Prof. Swapan K Pati (pati@jncasr.ac.in)

Academic Record

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

Peer Reviewed Publications

1. ***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

2. ***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

3. ***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

4. ***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

5. ***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

6. ***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

7. ***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

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. ***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

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

11. ***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

12. ***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

Preprints

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

2. ***Conformational Dynamics of the Pyrene Excimer***
   Giovanni Parolin, **Bidhan Chandra Garain**, Saikat Mukherjee, Giovanni Granucci, Stefano Corni, Mario Barbatti

3. ***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

Conference Presentations

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**.

Scholarships and Awards

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

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

The fellow has supervised a master's student at JNCASR, Utkarsh Singh, whose research has 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 will support Utkarsh Singh in the completion and submission of his master's thesis.

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), ***Quantum Dynamics codes*** (Multi Configuration Time Dependent Hartree (MCTDH), Qutip), ***Machine Learning and Deep Learning*** (Pytorch and Scikit-Learn) and ***Visualization*** (Matplotlib, Plotly and Seaborn), Git