SARTHAK MAITY

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Dhasachandpur, Mansuka, Ghatal, Paschim Medinipur, West Bengal, 721212, India

EDUCATION & TRAINING

Indian Institute of Technology Indore (IIT Indore) Aug 2023 – May 2025

M. Sc. in Chemistry (CGPA: 8.57/10.00) Advisor: Prof. Biswarup Pathak

Theoretical & Computational Chemistry

Midnapore Day College (Autonomous) Sep 2020 – Jun 2023

B. Sc. in Chemistry *(*HONS) (CGPA: 8.00/10.00)

Baradongal Ramanath Institution (10+2) 2018 – 2020

Physics, Chemistry, Mathematics, Biology (PCMB) (Score: 92.4/100)

SCHOLARSHIPS & AWARDS

Swami Vivekananda Merit-cum-Means Scholarship (SVMCM) 2018 – 2023

SCHOLASTIC ACHIEVEMENTS

Secured All-India Rank **504** (Chemistry) in Joint Admission Test for Masters (IIT JAM) 2023

Shortlisted for Integrated Ph.D. Interview, IISER Mohali (India) 2023

WORK & RESEARCH EXPERIENCE

Department of Chemistry, IIT Indore Aug 2024 – May 2025

Computational Material Design Group (CMDG) Postgraduate Researcher

Master Project: *Deciphering Key Descriptors for Scaling Relationships in Graphene-Supported Pt_n Clusters via Machine Learning*

Advisor: Prof. Biswarup Pathak

- An ensemble-based DFT framework that captures fluxionality by considering multiple low-energy isomers of subnanometer Pt clusters instead of a single static structure.
- An interpretable supervised ML model enabling accurate prediction of ORR intermediate adsorption energies.
- Descriptor-level identification of scaling-relation breakdown using uncertainty quantification, revealing the geometric features that control non-scalable ORR behavior in subnanometer catalysts.
- A coverage-dependent ORR activity analysis up to monolayer coverage, integrating ab initio oxidation thermodynamics and reaction network analysis under realistic electrochemical conditions.

Mini Project-I Aug 2023 – Oct 2023

Title: *Synthesis and Characterization of N-Containing Heterocyclic Compounds*

Supervisor: Prof. Umesh A. Kshirsagar, IIT Indore, India

- Developed synthetic routes for fused bicyclic and heterocyclic compounds relevant to drug design.
- Achieved synthesis of 4H-pyrido[1,2-a]pyrimidin-4-ones using β-keto esters and PPA.
- Performed Cu(I)-catalyzed oxidative synthesis of imidazo[1,2-a]pyridines in aqueous media.

Mini Project-II Oct 2023 – Feb 2024

Title: *Superior Anchoring Effect of Cu-Benzenehexathial MOF as an Al–S Battery Cathode Host*

Supervisor: Prof. Biswarup Pathak, IIT Indore, India

- Identified 2D Cu-BHT MOF as an efficient sulfur host cathode via DFT calculations.

- Demonstrated stronger binding of Al polysulfides compared to graphene-based hosts.
- Showed enhanced sulfur incorporation and reduced polysulfide dissolution, improving cycling stability.

Mini Project-III Feb 2024 – May 2024
Title: *Sequestration of Radioiodides Using Ionic Porous Organic Polymer*
Supervisor: Prof. Suman Mukhopadhyay, IIT Indore, India

- Designed and synthesized a multifunctional ionic porous organic polymer (iPOP-Bpy).
- Incorporated viologen as a redox-active unit to enhance iodine capture efficiency.
- Achieved high iodine uptake with rapid adsorption kinetics across gas and solution phases.

PUBLICATIONS

[1] co-first authorship; * corresponding author.

1. **Maity, S.**[1]; Sharma, R. K.[1]; Minhas, H.; Pathak, B.* *Deciphering Key Descriptors for Scaling Relationships in Graphene-Supported Pt Clusters via Machine Learning*. *small*, ***smll.202513283***, **2025**, submitted.

RESEARCH INTERESTS

- **Catalysis:** Realistic modeling of heterogeneous electrocatalysts, including dynamically evolving catalytic surfaces and interfaces under electrochemical reaction conditions.
- **Energy Storage:** Dual-ion, Al–S, and Li-ion batteries, electrolyte development and cathode material design.
- **Data-Driven Materials Design:** Structure–property modeling using graph neural networks and machine learning, DFT-trained neural network interatomic potentials, and inverse catalyst design via generative modeling (GenAI).

SKILLS

- **Atomistic ML Tools:** Machine Learning Interatomic Potentials (MLIPs): ALIGNN, MatGL, MACE
- **Programming Skills:** Graph Neural Networks (GNNs), Deep Learning (DGL, PyTorch, Keras), Machine Learning (Scikit-learn), Python (NumPy, Pandas, Matplotlib, Seaborn), LaTeX, FORTRAN
- **Software:** VASP, VESTA, Chemcraft, Gaussian, GaussView, ORCA, Materials Project, Materials Studio, OriginPro, ChemDraw
- **Office Tools:** MS Word, PowerPoint, Excel
- **Languages:** English, Hindi, Bengali

CERTIFICATIONS

- **Supervised Machine Learning: Regression and Classification**, DeepLearning.AI (Coursera), Dec 2025. Credential ID: 6FVINQX6DJK7. Certificate

CONFERENCES & SEMINARS

- In-house Symposium, Department of Chemistry, IIT Indore Mar 2024
- International Indo–German Conference on Sustainable Chemistry–III, IIT Indore Mar 2025