Dr. Sneha Mittal

CURRENT POSITION

Postdoctoral Fellow, Department of Physics - 2DPHYS, Technical University of Denmark (DTU), 2800 Kgs. Lyngby, Denmark **snemi@dtu.dk** | **snehamittalphd@gmail.com** | Google Scholar | ORCID

1. DOCTOR OF PHILOSOPHY (Ph.D.)

Overall CPI of the Course Work: 9.65

Thesis Title: Development of Single-Base Resolution Methods for Sequencing of Natural, Mutated, and Artificial DNA Using DFT and Machine Learning

Ph.D. Chemistry: 2020 (January) – 2024 (November) Department of Chemistry, Indian Institute of Technology Indore, India– 453552

PhD Supervisor: Prof. Biswarup Pathak, FNASc, FRSC, Associate Editor, ACS Applied Materials & Interfaces, IIT Indore

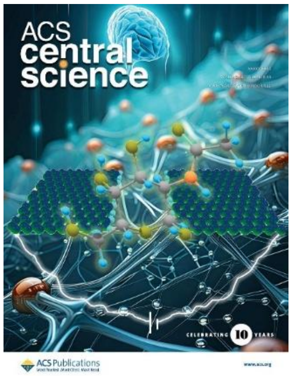
2. LIST OF PUBLICATIONS

List of patents

1. Biswarup Pathak, **Sneha Mittal**, Milan Kumar Jena, Method and System for Identifying Disaccharide Isomers thereof; Indian Patent *E-106/5190/2024/MUM* (Filed)
2. Biswarup Pathak, Milan Kumar Jena, **Sneha Mittal**, Method and System for Identifying a Molecule of Artificial Deoxyribonucleic Acid (DNA) thereof; Indian Patent *E-106/104/2025/MUM* (Filed)

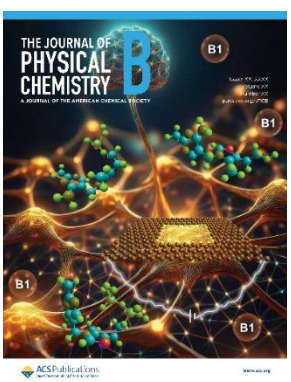
List of publications

1. **Mittal, S.**, Jena, M. K., Pathak, B. (2024) Integration of artificial Intelligence and quantum transport towards stereoselective identification of carbohydrate isomers, **ACS Cent. Sci.**, 10, 9, 1689–1702 | Front Cover Article **(Impact Factor: 10.4)**



2. **Mittal, S.**, Manna, S., Jena, M.K., Pathak, B. (2023), Decoding both DNA and methylated DNA using a MXene-based nanochannel device: supervised machine-learning-assisted exploration, **ACS Materials Lett.**, 5, 1570–1580. (DOI: 10.1021/acsmaterialslett.3c00117) **(Impact Factor: 8.7)**
3. **Mittal, S.**, Manna, S., Pathak, B. (2022), Machine learning prediction of the transmission function for protein sequencing with graphene nanoslit, **ACS Appl. Mater. Inter.**, 14, 51645–51655. (DOI: 10.1021/acsami.2c13405) **(Impact Factor: 8.2)**
4. **Mittal, S.**, Jena, M. K., Pathak, B. (2024), Machine learning empowered next generation DNA sequencing: perspective and prospectus, **Chem. Sci.,** 15, 12169-12188 | Perspective **(Impact Factor: 7.4)**
5. **Mittal, S.**, Jena, M. K., Pathak, B. (2024), Machine learning assisted direct RNA sequencing with epigenetic RNA modifications detection via quantum tunneling, **Anal. Chem.,** 96, 28, 11516–11524 | Front Cover Article **(Impact Factor: 6.7)**

6. **Mittal, S.**, Pathak, B. (2023), Towards a graphene semi/hybrid-nanogap: a new architecture for ultrafast DNA sequencing, **Nanoscale**, 15, 757–767. (DOI: 10.1039/D2NR05200H) **(Impact factor: 6.7) (Impact Factor: 5.1)**
7. **Mittal, S.**, Manna, S., Jena, M.K., Pathak, B. (2023), Artificial intelligence aided recognition and classification of DNA nucleotides using MoS_2 nanochannels, **Digit. Discov.**, 2, 1589–1600. (DOI: 10.1039/D3DD00118K) **(Impact Factor: 5.6)**
8. **Mittal, S.**, Jena, M.K., Pathak, B. (2022), Amplifying quantum tunneling current sensitivity through labeling nucleotides using graphene nanogap electrodes, **ACS Appl. Nano Mater.**, 5, 9356–9366. (DOI: 10.1021/acsanm.2c01667) **(Impact Factor: 5.5)**
9. **Mittal, S.**, Kumawat, R. L., Jena, M. K., Pathak, B., (2022), Graphene nanoslit device for protein sequencing: ab initio quantum transport study, **ACS Appl. Nano Mater.** 5, 2715–2727. (DOI: 10.1021/acsanm.1c04369) **(Impact Factor: 5.5)**
10. **Mittal, S.** & Pathak, B., (2023), A step toward amino acid-labeled DNA sequencing: boosting transmission sensitivity of graphene nanogap, **ACS Appl. Bio Mater.** 6, 218–227. (DOI: 10.1021/acsabm.2c00851) **(Impact Factor: 4.7)**
11. **Mittal, S.**, Jena, M. K., Pathak, B. (2023), Protein sequencing with artificial intelligence: machine learning integrated phosphorene nanoslit, **Chem. Eur. J.** 29, e202301667 (DOI: 10.1002/chem.202301667) **(Impact Factor: 3.7)**
12. **Mittal, S.**, Jena, M. K., Pathak, B. (2025), Automated-screening oriented electric sensing of vitamin B1 using artificially intelligent solid-state nanopore, **J. Phys. Chem. B**, 129, 4, 1301–1310 (DOI: 10.1021/acs.jpcb.4c05619) **(Impact Factor: 2.9)**



13. **Mittal, S.,** Jena, M. K., Pathak, B. Unlocking the 12-Letter Genetic Code: ML-Empowered Quantum Nanopore Base-Calling Even for DNA Isomers, **ACS Appl. Nano Mater.** 2025, 8, 23, 12065–12078 **(Impact Factor: 5.5)**

14. Kumawat, R. L., Jena, M. K.*, **Mittal, S.***, Pathak, B. (2024), Advancement of next-generation DNA sequencing through ionic blockade and transverse tunneling current methods. **Small**, 2401112. (DOI: 10.1002/smll.202401112) | Review Article **(Impact Factor: 12.1)**
15. Jena, M. K., Roy, D., **Mittal, S.**, Pathak, B. (2023), Artificially intelligent nanogap for rapid DNA sequencing: a machine learning aided quantum tunneling approach. **ACS Materials Lett.** 5, 2488–2498. (DOI: 10.1021/acsmaterialslett.3c00475) **(Impact Factor: 8.7)**
16. Jena, M. K., **Mittal, S.**, Pathak, B. (2024), Precision basecalling of single DNA nucleotide from overlapped transmission readouts with machine learning aided solid-state nanogap, **ACS Appl. Mater. Interfaces** (DOI: 10.1021/acsami.4c04858) **(Impact Factor: 8.2)**
17. Maurya D.; **Mittal, S.**, Jena, M. K., Pathak, B. Machine Learning Driven Quantum Sequencing of Natural and Chemically Modified DNA, **ACS Appl. Mater. Interfaces** 2025 (Just Accepted) **(Impact Factor: 8.2)**
18. Jena, M. K., **Mittal, S.**, Manna, S. S., Pathak, B. (2023), Deciphering DNA nucleotide sequences and their rotation dynamics with interpretable machine learning integrated C_3N nanopores. **Nanoscale**, 15, 18080–18092. (DOI: 10.1039/D3NR03771A) **(Impact Factor: 5.1)**
19. Pandit, S., Jena, M. K., **Mittal, S.**, Pathak, B. (2024), Machine learning prediction and classification of transmission functions for rapid DNA sequencing in a hybrid nanopore, **ACS Appl. Nano Mater.**, 7, 14, 17120–17132 (DOI: 10.1021/acsanm.4c03685) **(Impact Factor: 5.5)**
20. Mukherjee, S., Chandrashekar, P., Aby, I. E., **Mittal, S.**, Varghese, A., Pathak, B., Mandal, S. (2023), Quasi-isomeric anion-templated silver nanoclusters: effect of bulkiness on luminescence, **J. Phys. Chem. Lett.** 14, 8548– 8554. (DOI: 10.1021/acs.jpclett.3c02234) **(Impact Factor: 4.6)**
21. Rashid, M., Jena, M. K., **Mittal, S.**, Pathak, B. (2024), Effect of Graphene Electrode Functionalization on Machine Learning-Aided Single Nucleotide Classification, **Nanoscale**,16, 20202-20215 (DOI: 10.1039/d4nr02274b) **(Impact Factor: 5.1)**
22. Jena, M. K., **Mittal, S.**, Pathak, B. (2025), Machine Learning Recognition of Artificial DNA Sequence with Quantum Tunneling Nanogap Junction, **J. Phys. Chem. B,** 129, 3, 853–865 (DOI: 10.1021/acs.jpcb.4c06270) **(Impact Factor: 2.9)**

23. Parveen, D., **Mittal, S.**, Shrivas R., Pathak, B. Roy, D., K. Hydrophosphinylation of Alkynes via Magnesium Complexes: Evidence for Ligand Dependency in Structure-Activity Relationships, **Chem. Eur. J.** 2025, e202500002 (DOI: 10.1002/chem.202500002 **(Impact Factor: 3.7)**

Manuscripts Under Communication

24. **Mittal, S.,** Jena, M. K., Pathak, B. Hybrid Supervised and Unsupervised Machine Learning Approach for Identifying Nucleoside Drugs Using Nanopore Readouts (*Revision submitted*)
25. **Mittal, S.**, Jena, M. K., Pathak, B. Decoding Regioselectivity of Disaccharides using Quantum Transport and Artificial Intelligence (*Under Review*)
26. **Mittal, S.**, Jena, M. K., Pathak, B. Unveiling Amino Acid Variants: Data-Driven Recognition of Enantiomers and Post-Translational Modifications via Quantum Tunneling (*Manuscript Prepared*)
27. **Mittal, S.**, Jena, M. K., Pathak, B. Unsupervised Clustering of DNA Transmission Footprints Using Single-Layer MoS_2/WSe_2 Heterojunction (*Under Review*)
28. Chatterjee D.; **Mittal, S.**, Jena, M. K., Pathak, B. Machine Learning Boosted Quantum-Profiling of Blood Antigens and Lewis Trisaccharides *(Under Review)*
29. Rashid, M., Jena, M. K., **Mittal, S.**, Pathak, B. Quantum Transport-Informed Machine Learning Mapping of Current-Voltage Characteristics for Precision DNA Sequencing (*Under Communication*)

3. AWARDS/RECOGNITION RECEIVED

- **Young Theoretical Chemist Association Scholarship** from TACC 2023 International Conference, Hokkaido University, Japan — 2023
- **Best Poster Presentation Award,** TACC 2023 International Conference, Hokkaido University, Japan — 2023
- **CSIR International Travel Grant (Govt. of India)** to Attend TACC 2023 Conference, Hokkaido University, Japan (4^{th}-9^{th} — 2023

September)

- **Best Oral Presentation Award** from International Conference on Sustainable Chemistry-2023, under INDO-GERMAN Higher Education Partnership, IIT Indore — 2023
- **Best Oral Presentation Award** from TECHNO SAMVAD Events, IIT Indore — 2023
- Qualified **CSIR-NET (JRF)** with All India Rank-40 — 2019
- Awarded **DST INSPIRE Scholarship**, Govt. of India — 2013-2018
- **Bal Ratna-Khoj-**Kabir Peace Mission Award — 2011
- **Rajya Puraskar Award** – *The Bharat Scouts and Guides* — 2010

Conferences/workshops attended

- Certificate of Hyderabad-Heidelberg Hub for Advanced Chemical Education **(H3ACE) workshop**, IIT Hyderabad — 2025
- Certificate of oral presentation, **EESTER conference**, SRM-IIT Madras — 2023
- Certificate of poster presentation, **EMEE conference**, IIT Roorkee — 2023
- Certificate of poster presentation, **TCS conference**, IIT Madras — 2023

4. ORGANIZED ANY DEPARTMENTAL ACTIVITY (AS AN ORGANIZING TEAM)

- Volunteered (Anchoring) for "**Sustainable Chemistry IGP conference** under INDO-GERMAN Higher Education Partnership", Department of Chemistry, IIT Indore — 2023
- Volunteered (Anchoring) for "**In-House Symposium: CHEM**" Department of Chemistry, IIT Indore — 2020
- Volunteered for "**National Science Day**"- Chemical Illusion Experiment, Department of Chemistry, IIT Indore — 2020

5. NOVELTY OF THE THESIS

The thesis introduces an "*AI-integrated quantum transport*" approach, revolutionizing next-generation DNA sequencing by merging quantum transport methods with explainable artificial intelligence (AI) tools. This innovative framework dramatically enhances precision and throughput in DNA sequencing, enabling single-nucleotide resolution across genomics, epigenomics, and artificial genomics. Utilizing first-principles DFT and machine learning, it accurately identifies diverse DNA nucleobases, including isomers and critical cancer biomarkers, addressing a core challenge in chemistry and biology. This methodology not only reduces costs and operational time but also sets a new standard for high-throughput, automated, and interpretable molecular diagnostics while also uniquely enabling chiral discrimination.

6. SOCIAL IMPACT OF THE PH.D. THESIS

The thesis holds a profound social impact by transforming DNA sequencing into a faster, more accurate, and cost-effective process, with wide-reaching benefits in healthcare, diagnostics, and personalized medicine. By enabling precise detection of genetic disorders and cancer biomarkers with single-nucleotide resolution, the approach empowers preventative care and targeted therapies, especially in underserved populations. Its high-throughput, automated nature enhances global accessibility to genomic technologies. Moreover, its explainable AI integration fosters transparency and trust in clinical decision-making. The ability to detect subtle molecular variations, including chiral isomers, opens new avenues in drug development, environmental monitoring, and biosafety, significantly advancing public health and societal well-being.

7. SCIENTIFIC IMPACT OF THE PH.D. THESIS

The thesis delivers a significant scientific breakthrough by integrating quantum transport methods with explainable AI, offering a novel and interdisciplinary framework for molecular recognition at the atomic scale. It advances the frontier of DNA sequencing by achieving single-nucleotide and isomer-level resolution, addressing longstanding challenges in molecular identification, chiral discrimination, and label-free sensing. By leveraging first-principles density functional theory (DFT) and machine learning, the work advances automated data interpretation and base-calling accuracy in DNA sequencing. This research sets a new benchmark in computational biophysics and quantum chemistry, fostering innovations in genomics, biosensing, and AI-driven materials science, and opening pathways for future quantum-biological technologies.