

Dr. Rabindra Nath Manna
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Work Experience

- Nov 2023 – Present: **Assistant Professor, Ghatal Rabindra Satabarsiki Mahavidyalaya.**
- Aug 2023 – Nov 2023: **Project Scientist D, S. N. Bose National Centre for Basic Sciences.**

Postdoc Research Experience

- Sept 2022 – Aug 2023: **Research Associate I and II, Indian Association for the Cultivation of Science, India.** (Supervisor: Prof. Debashree Ghosh)
- Sept 2019 – Sept 2022: **Research Associate I, Indian Association for the Cultivation of Science, India.** (Supervisor: Prof. Ankan Paul)
- Nov 2015 – Aug 2019: **Research Associate I, National Postdoctoral Fellow, Indian Association for the Cultivation of Science, India.** (Supervisor: Prof. Biman Jana)

Education

- **Ph.D (2015), Lodz University of Technology, Poland.**
Ph.D Thesis Title: “Theoretical study on aerobic degradation processes of hexachlorocyclohexane isomers catalyzed by the haloalkane dehalogenases LinA and LinB” (Supervisor: Dr. Agnieszka Dybala-Defratyka).
- **M.Sc (2010), Indian Institute of Technology Bombay.**
Master Thesis Title: “Computational design of organocatalysis for stereoselective aldol reaction.” (Supervisor: Prof. R. B. Sunoj). Subject: Chemistry.
- **B.Sc (2008), University of Calcutta, India.**

Research visits

- 2014, **University of Bath, UK.** Supervisor: Prof. Ian H. Williams. (Predict ensemble-averaged isotope effects for the condensed phase systems)
- 2014, **University of Valencia, Spain,** Supervisor: Prof. Iñaki Tuñón. (Free energy enhanced sampling MD simulations techniques)

List of Publications

1. S. Moyra; T. N. Das; **R. N. Manna**; G. Ghosh, Tuning Supramolecular Polymerization and Pathway Complexity via Spacer Length-Directed Molecular Angles in Pyrene-Conjugated Peptides, *Polym. Chem.* 2026, Link : <https://doi.org/10.1039/D6PY00525J> ISSN: 1759-9962, **Impact factor: 3.9.**
2. R. Nath, S. Panja, **R. N. Manna**, A. Paul, Elucidating the Molecular Determinants of Substrate Specificity in salicylate 1,2 deoxygenate: A QM/MM Investigation of Salicylate and Gentisate, *The Journal of Physical Chemistry B*, 2026, (just accepted) ISSN 1520-6106, **Impact factor: 2.9.**
3. S. Santra, **R. N. Manna**, S. Chakrabarty, D. Ghosh, “Conformational Effects on the Absorption Spectra of Phytochromes”, *The Journal of Physical Chemistry B*, 2024, 128, 3614-3620. ISSN 1520-6106, **Impact factor: 2.9.**
4. A. Ghosh, M. Mondal, **R. N. Manna**, A. Bhaumik, “Targeted synthesis of a metal-free thiadiazolate based nitrogen and sulfur rich porous organic polymer for an unprecedented hydrogen evolution in the electrochemical water splitting”, *Journal of Colloid and Interface Science*, 2024, 658, 415-424. ISSN 1095-7103, **Impact Factor: 9.7.**
5. **R. N. Manna**, J. N. Onuchic. B. Jana, “Second Sphere Control of Pre-Organization for ATP Hydrolysis in Kinesin: Rationale for Hereditary Spastic Paraplegia Disease,” *Proceedings of the National Academy of Sciences U.S.A.* 2022, 120, e2215170120. ISSN 1091-6490 . **Impact Factor 12.78.**
6. R. Khamrui, **R. N. Manna**, P. Rajdev, A. Paul, S. Ghosh. “Impact of the Hydrogen-Bonding Functional Group on Hydrogelation of Amphiphilic Naphthalene-diimide Derivatives and Non-specific Protein Adsorption,” *ACS Applied Bio Materials*, 2022, 5, 5410-5417. ISSN 2576-6422.

7. R. Nath[#], **R. Manna[#]**, A. Paul, “Decoding Regioselective Reaction Mechanism of the Gentisic Acid Catalyzed by Gentisate 1,2-Dioxygenase Enzyme. Catalysis,” *Catalysis Science & Technology*, 2022, 12, 5742-5751. ISSN 2044-4761. **Impact factor 6.177.** ([#] contributed equally)
8. A. Ghosh, S. Shymal, A. Palui, **R. N. Manna**, M. Jana, S. Mandal, A. Ghosh, A. Bhaumik, “Photoelectrochemical Water oxidation of a Novel Semiconductive Zinc based Metal Thiolate Frameworks,” *ACS Applied Materials & Interfaces*, 2022, 14, 37699–37708. ISSN 1944-8244. **Impact factor 10.38.**
9. B. Ghosh, A. Banerjee, L. Roy, **R. N. Manna**, R. Nath, A. Paul. “The Role of Copper Salts and O₂ in the Mechanism of C≡N Bond Activation for Facilitating Nitrogen Transfer Reactions”. *Angewandte Chemie*, 2022, 61, e202116868. ISSN 1521-3773. **Impact Factor 15.34.**
10. A. Chakraborty, **R. N. Manna**, A. Paul, S. Ghosh, “Externally Regulated Specific Molecular Recognition Driven Pathway Selectivity in Supramolecular Polymerization”. *Chemistry – A European Journal*, 2021, 27, 11458-11467, ISSN 1521-3765, **Impact Factor 5.236.**
11. A. Pradhan, R. N. Manna, “Surface-Modified Covalent Organic Polymer for Metal-Free Electrocatalytic Hydrogen Evolution Reaction”. *ACS Applied Polymer Materials*, 2021, 3, 1376–1384, ISSN 2637-6105, **Impact Factor 4.089.**
12. A. Sowińska, L. Vasquez, S. Żaczek, **R. N. Manna**, I. Tuñón, A. Dybala-Defratyka, “Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA”. *The Journal of Physical Chemistry B*, 2020, 124, 10353–10364, ISSN 1520-5207, **Impact Factor 2.991.**
13. D. Mukherjee, **R. N. Manna**, P. Saha, U. Mandal, M. Mitra, “Electronic and Molecular Characterization of An Air-stable Cr (II) Complex Containing Azo-Anion-Radicals”. *Journal of Molecular Structure*, 2020, 1223, 129247-129255. ISSN 0022-2860, **Impact factor 3.196.**
14. **R. N. Manna**, M. Dutta, B. Jana, “Mechanistic Study of ATP Hydrolysis Reaction in Dynein Motor Protein”. *Physical Chemistry Chemical Physics*, 2020, 22, 1534-1542. ISSN 1463-9084, **Impact factor 3.676.**
15. **R. N. Manna[#]**, T. Malakar,[#] B. Jana, A. Paul, “Unraveling the Crucial Role of Single Active Water Molecule in the Oxidative Cleavage of Aliphatic C–C Bond of 2,4'-Dihydroxyacetophenone Catalyzed by 2,4'-Dihydroxyacetophenone Dioxygenase Enzyme: A Quantum Mechanics/Molecular Mechanics Investigation”. *ACS Catalysis* 2018, 8, 10043-10050. ISSN 2155-5435, **Impact factor 13.086.** ([#]contributed equally)
16. **R. N. Manna**, A. Grzybowska, F. Gelman, A. Dybala-Defratyka, “Carbon-bromine bond cleavage—A perspective from bromine and carbon kinetic isotope effects on model debromination reactions”. *Chemosphere*, 2018, 193, 17-23. ISSN 0045-6535, **Impact factor 7.086.**
17. B. C. Patra, S. Khilari, **R. N. Manna**, S. Mondal, D. Pradhan, A. Pradhan, A. Bhaumik, “A Metal-Free Covalent Organic Polymer for Electrocatalytic Hydrogen Evolution”. *ACS Catalysis*, 2017, 7, 6120-6127. ISSN 2155-5435, **Impact factor 13.084.**
18. R. Halder, **R. N. Manna**, S. Chakraborty, B. Jana, “Modulation of the Conformational Dynamics of Apo-Adenylate Kinase through a π -Cation Interaction”. *The Journal of Physical Chemistry B* 2017, 121, 5699-5708. ISSN 1520-5207, **Impact factor 2.991.**
19. L. Szatkowski,* **R. N. Manna,*** A. Grzybowska,* R. Kamiński, A. Dybala-Defratyka, P. Paneth, “Measurement and Prediction of Chlorine Kinetic Isotope Effects in Enzymatic Systems”. *Methods in Enzymology*, 2017, 596, 179-215. (*contributed equally) ISSN 0076-6879, **Impact factor 2.002.**
20. P. Maity, S. Ahammed, **R. N. Manna**, B. C. Ranu, “Calcium mediated C–F bond substitution in fluoroarenes towards C–chalcogen bond formation”. *Organic Chemistry Frontiers*. 2016, 4, 69-76. ISSN 2052-4129, **Impact factor 5.281.**
21. S. Parui, **R. N. Manna**, B. Jana, “Destabilization of Hydrophobic Core of Chicken Villin Headpiece in Guanidinium Chloride Induced Denaturation: Hint of π -Cation Interaction”. *The Journal of Physical Chemistry B* 2016, 120, 9599-9607. ISSN 1520-5207, **Impact factor 2.991.**
22. **R. N. Manna**, K. Zinovjev, I. Tuñón, A. Dybala-Defratyka, “Dehydrochlorination of Hexachlorocyclohexanes Catalyzed by the LinA Dehydrohalogenase. A QM/MM Study”.

The Journal of Physical Chemistry B 2015, 119, 15100-15109. ISSN 1520-5207, **Impact factor 2.991**.

23. **R. N. Manna**, A. Dybala-Defratyka, "A computational study of the dechlorination of β -hexachlorocyclohexane (β -HCH) catalyzed by the haloalkane dehalogenase LinB". **Archives of Biochemistry and Biophysics**. 2014, 562, 43-50. ISSN 0003-9861, **Impact factor 4.031**.
24. **R. N. Manna**, A. Dybala-Defratyka, "Insights into the elimination mechanisms employed for the degradation of different hexachlorocyclohexane isomers using kinetic isotope effects and docking studies". **Journal of Physical Organic Chemistry**, 2013, 26, 797-804. ISSN 1099-1395, **Impact factor 2.391**.

Conferences

- **8th Regional Science & Technology Congress 2025-26, WBDST**, Debra Thama Sahid Kshudiram Smriti Mahavidyalaya, R. N. Manna, Integrating Cheminformatics and Machine Learning to Predict BACE1 Inhibitors from ChEMBL.
- **Femex 2014 in Oslo, Norway**. R. N. Manna, A. Dybala-Defratyka. "A QM/MM study on the dehalogenation reaction of the hexachlorocyclohexane (HCH) isomers catalyzed by LinA and LinB dehalogenases".
- **MDMM 2014, Kudowa Zdroj, Poland**. R. N. Manna, A. Dybala-Defratyka. "A QM/MM study on the dehalogenation reaction of the hexachlorocyclohexane (HCH) isomers catalyzed by LinA and LinB dehalogenases".
- **ISOTOPES 2013, Sopot, Poland**. R. N. Manna, A. Dybala-Defratyka. "Theoretical modeling of kinetic isotope effects on aerobic degradation of hexachlorocyclohexane isomers catalyzed by LinA and LinB".
- **Gordon Research Conference 2012, Galveston, USA**. R. N. Manna, A. Dybala-Defratyka, P. Paneth. "Kinetic isotope effects on elimination pathways employed for degradation of different hexachlorocyclohexanes isomers".
- **ISOTOPES 2011, Greoux-les-Bains, France**. R. N. Manna, A. Dybala-Defratyka, P. Paneth. "Probing the degradation mechanism of γ -hexachlorocyclohexane by LinA enzyme".

Professional Training

- 25/08/2025-22/09/2025: "2nd Faculty Induction Programme, **UGC-Malaviya Mission Teacher Training Programme, University of Burdwan**.
- 17/03/2019-22/03/2019: "Workshop on Free energy calculations for chemical and biological systems" **IIT Kanpur**.
- 24/06/2013-28/06/2013: "Course on molecular modeling" **Lodz University of Technology, Poland**.
- 16/04/2013-19/04/2013: "Reactive transport modeling of isotope signals in the environment" **VU University of Amsterdam, Netherland**.
- 12/11/2012-14/11/2012: "Course on N isotope methods" **EWAG-ETH, Switzerland**.
- 10/09/2012-14/09/2012: "Course on modern methods and applications for isotope analysis of light elements" **Helmholtz Centre for Environmental Research-UFZ, Germany**.
- 6/05/2012-12/05/2012: "Course on halogen and radiocarbon isotopes in geochemistry" **Stockholm University, Sweden**.
- 20/02/2012-22/02/2012: "Course on ISO-QA assuring the quality of isotopic data used for environmental applications" **CSIC Barcelona, Spain**.
- 15/02/2012-18/02/2012: "Course on analytical methods" **CSIC Barcelona, Spain**.
- 31/03/2011: **Schrödinger Workshops** "Computational drug discovery- exploring various approaches for novel hit identification" **ICM Warsaw, Poland**.

Scholarships and Awards

- SERB-National Postdoctoral fellowship (NPDF): 2017-2019
- Foreign PhD Scholarship, Lodz University of Technology: 2013-2015.
- **European Marie Skłodowska-Curie actions CSI-ITN fellowship: 2011-2014**.
- CSIR-NET in Chemistry: 2010.

- GATE in Chemistry: 2010
- IIT JAM: 2008.