# Manabendra Sarma

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**Name** Manabendra Sarma

**Sex** Male

**Date of Birth** 30 June, 1979

**Place of Birth** Ratanpur, Nalbari, Assam, India

**Nationality** Indian (by birth)

**Languages** English, Hindi, Assamese (read, write and speak)

**Positions Held**

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|---|---|---|
| Professor | December 11, 2024 – Present | I I T Guwahati |
| Associate Professor | February 21, 2015 – December 10, 2024 | I I T Guwahati |
| Assistant Professor | April 01, 2009 – February 20, 2015 | I I T Guwahati |
| Senior Lecturer | August 2008 – November 2008 | I I T Patna (on deputation) |
| Senior Lecturer | May 15, 2008 – March 31, 2009 | I I T Guwahati |
| Junior Research Fellow (BRNS Project) | February 01, 2008– May 14, 2008 | I I T Bombay |
| CSIR Senior Research Fellow | February 2005 – January 2008 | I I T Bombay |
| CSIR Junior Research Fellow | February 2003 – January 2005 | I I T Bombay |
| Junior Research Fellow (DST Project) | September 2002 – January 2003 | I I T Bombay |

**Education**

- **Post-Doctoral Fellow**, **University of Heidelberg**, Germany, 2011 – 2012
  **Supervisor :** Professor Lorenz S. Cederbaum
- **Ph. D.** (Theoretical Chemistry), **IIT Bombay,** Mumbai, 2002 – 2008
  **Thesis Supervisor :** Professor Manoj K Mishra
- **M. Sc.** (Chemistry), **IIT Guwahati**, Guwahati, 2000 – 2002
  **Project Supervisor :** Professor Anumita Paul

- **B. Sc.** (Chemistry)**, Goalpara College,** Goalpara, Assam with English, Physics and Mathematics, 1997 – 2000

**Research Interests**

Development of new theoretical approaches to:

- Laser Assisted Control of Chemical Reactions,
- Resonances in Electron – Molecule Scattering
- Electronic Structure Theory and Quantum Molecular Dynamics of Small to Large Systems

**Awards & Honors**

- **Fellow of the Royal Society of Chemistry (FRSC), December 2020**
- **BOYSCAST Fellowship** for the year 2010 – 2011 at the **University of Heidelberg, Germany** under **Professor Lorenz S. Cederbaum**
- **CSIR Senior Research Fellowship**, February 2005 – January 2008
- **CSIR Junior Research Fellowship**, February 2003 – January 2005
- **Graduate Aptitude Test in Engineering (GATE)** Qualified, 2002

**Membership of Scientific Societies/Bodies**

- **Member, American Chemical Society (ACS), August 2020**
- **Life Member of Chemical Research Society of India (CRSI), May 2020**
- **Member of the Royal Society of Chemistry (MRSC), April 2019**
- **Associate Member of the Royal Society of Chemistry (AMRSC), November 2018**

**Editorial Board Member**

- **Guest Editor,** jointly with Dr. Amrit Sarmah, Dr. Rabindranath Lo, and Dr. Debashree Manna for a **Special Issue on "Expanded Porphyrin Chemistry: The Recent Advances and Promising Future Trends"** of the journal ***Molecules*, MDPI, (2022)** [https://www.mdpi.com/journal/molecules/special_issues/2193C3VH2R].

**Research Publications in Refereed Journals** [* Corresponding Author]

1. M. Sarma and **M. Sarma***, "Synergistic Use of Molecular Dynamics Simulations and Quantum Mechanical Approaches to Unveil the Peptide-Arsenic Interactions", (in preparation).

2. B. Lama and **M. Sarma*** (2025), "Photodynamics Simulation Insights into Excited-State Relaxation Mechanisms via Z/E Isomerization in Para-Amino Substituted GFP Chromophores", J. Chem. Phys. **163**, 054305 (1 – 13).

3. S. Kumar, M. P. Sarmah, P. Dash, and **M. Sarma*** (2025), "Study of Electron Capture by 5-Halogenated Cytosine in Gas and Condensed Phases", J. Phys. Chem. A **129**, 7429 – 7439.

4. U. Nath and **M. Sarma*** (2025), "$CO_2$ Activation and Electrochemical Reduction to $CH_3OH$ via Charge Modulation on Defect-Induced Freestanding Bilayer Borophene", J. Phys. Chem. C **129**, 13939 – 13953.

5. S. K. Bora, B. Medhi, **M. Sarma**, and **A. K. Saikia*** (2025), "A $BF_3 \bullet OEt_2$ Mediated Cascade Synthesis of 4H-3,1-Benzoxazines from 2-Azidobenzaldehydes and Homoallylic Alcohols", J. Org. Chem. **90**, 6443 – 6453.

6. M. Sarma, J. Dutta, and **M. Sarma*** (2025), "Deciphering the Underlying Mechanism of Anion Binding by Asymmetrical Squaramide-based Dipeptides", J. Phys. Chem. B **129**, 4949 – 4961 (**This article has appeared as a Cover Feature of the Journal**).

7. R. R. Changmai, S. R. Daimari, and **M. Sarma*** (2025), "Unveiling the Atmospheric Oxidation of Hexafluoroisobutylene, $(CF_3)_2C=CH_2$, with Cl atom, $NO_3$ radical, and $O_3$ molecule", J. Phys. Chem. A **129**, 3906 – 3920.

8. S. Shill, G. Dolai, R. R. Changmai, **M. Sarma**, and **B. Mandal*** (2025), "Unprecedented Binding of Thioflavin T with Well-Ordered Spherical Aggregates: A False Positive?", Spectrochim. Acta A **338**, 126165 (1 – 15).

9. N. Kalita, U. Nath, A. Singha, **M. Sarma**, and **M. Qureshi*** (2025), "Electronic Structure Tuning to Facilitate Charge Transfers in Z- Scheme Mediated CuO/Se@$WO_3$ aided by Synchronized $Cu(OH)_2$ for Efficient Overall Water Splitting", J. Mater. Chem. A **13**, 10723 – 10735.

10. D. Bora, F. R. Gayen, H. P. Bhattacharyya, S. Baguli, P. Patel, **M. Sarma***, and **B. Saha*** (2025), "Bimetallic Cooperativity of a Ferrocene-based Iridium NHC Complex in Water Oxidation Catalysis: A New Frontier for Efficient Oxygen Evolution", Chem. Asian J. **20**, e202401357 (1 – 10).

11. **Md. A. Alam***, A. Hoque, Md. S. Islam, N. Khatun, M. P. Sarmah, **A. K. M. Maidul Islam***, **M. Sarma***, **G. K. Kole***, and **E. Zangrando*** (2025), "An Electrically Conductive Dinuclear Aluminium Complex for the Fabrication of Schottky Diode", RSC Adv. **15**, 2132 – 2139.

12. A. Kalita, R. R. Changmai, **M. Sarma***, and **M. D. Saikia*** (2025), "Experimental and Computational Validation on the Adsorption Behaviour of Quercetin and Rutin on Ion Exchange Resins", Res. Surf. Interf. **18**, 100377 (1 – 13).

13. M. Sarma, M. P. Sarmah, and **M. Sarma*** (2025), "End Group Effects on Anion Binding in Tetraglycine Peptide: A Computational Study", Chem. Asian J. **20**, e202400880 (1 – 10).

14. H. P. Bhattacharyya and **M. Sarma*** (2024), "Role of Active Centers in Predicting the Catalyst Turnover: A Theoretical Study", Chem. Eur. J. **30**, e202403631 (1 – 10) (**This article has appeared as a Cover Feature of the Journal**).

15. M. P. Sarmah and **M. Sarma*** (2024), "Mechanistic Insights into the Electron Attachment Process to Guanosine in the presence of Arginine", Phys. Chem. Chem. Phys. **26**, 27955 – 27963.

16. N. Keot and **M. Sarma*** (2024), "Unraveling the Stability and Magnetic Properties of Bis-Hydrated Mn(II) Complexes via Tailored Ligand Design", J. Phys. Chem. A **128**, 8346 – 8359.

17. S. Kumar and **M. Sarma*** (2024), "Dissociative Electron Attachment to the Halogenated Nucleotides: A Quest for better Radiosensitizer", Phys. Chem. Chem. Phys. **26**, 25524 – 25532.

18. R. R. Changmai, S. R. Daimari, A. K. Yadav, and **M. Sarma*** (2024), "Atmospheric Oxidation Pathways of $CF_3CH_2CFCl_2$ (HCFC-234fb) with OH-Radical and Cl-Atom: Insights into Mechanism, Thermodynamics, and Kinetics", Phys. Chem. Chem. Phys. **26**, 23363 – 23371.

19. H. P. Bhattacharyya and **M. Sarma*** (2024), "MaxKinEff: A Collision Theory-Based Approach for Analyzing Turnover Frequency and Turnover Number in Catalytic Processes", Chem. Asian J. **19**, e202400674 (1 – 11).

20. S. R. Daimari, R. R. Changmai, and **M. Sarma*** (2024), "Investigating the Atmospheric Fate and Kinetics of OH Radical-Initiated Oxidation Reactions for Epoxybutane Isomers: Theoretical Insight", J. Phys. Chem. A **128**, 6240 – 6253.

21. B. Lama and **M. Sarma*** (2024), "Ultrafast Hot Exciton Nonadiabatic Excited-State Dynamics in Green Fluorescent Protein Chromophore Analogue", J. Phys. Chem. B **128**, 6786 – 6796.

22. T. Jena, Md. T. Hossain, U. Nath, **M. Sarma**, and **P. K. Giri*** (2024), "Salt-Catalyzed Directed Growth of Bilayer Palladium Diselenide ($PdSe_2$) Dendrites and $PdSe_2$-$Pd_2Se_3$ Junctions Exhibiting Very High SERS Sensitivity", Chem. Mater. **36**, 5922 – 5934.

23. **B. K. Rajbongshi***, S. Abdullah, B. Lama[#], H. P. Bhattacharyya[#], and **M. Sarma*** (2024), "Regioselective and Solvent-Dependent Photoisomerization Induced Internal Conversion in Red Fluorescent Protein Chromophore Analogues", RSC Adv. **14**, 18373 – 18384. [# Equal Contribution]

24. H. P. Bhattacharyya and **M. Sarma*** (2024), "Efficiency Conceptualization Model: A Theoretical Method for Predicting the Turnover of Catalysts", ChemPhysChem **25**, e202400004 (1 – 12).

25. B. Medhi, U. Nath, and **M. Sarma*** (2024), "Revisiting Fulgide Photochromism: Mechanistic Decoding and Electron Transport from Computational Exploration", J. Chem. Phys. **160**, 154308 (1 – 11).

26. U. Nath and **M. Sarma*** (2024), "Realization of Efficient and Selective NO and $NO_2$ Detection via Surface Functionalized h-$B_2S_2$ Monolayer", Phys. Chem. Chem. Phys. **26**, 12386 – 12396 (**Editors Choice 2024 HOT PCCP Article**).

27. **A. Sarmah***, M. Sarma, T. Nakajima, **M. Sarma**, and P. Hobza (2024), "Spintronics on Demand: Optically Tunable Kondo-type Phenomena in Germanene-Azobenzene Single-molecule Junction", J. Phys. Chem. C **128**, 4687 – 4698.

28. B. Medhi and **M. Sarma*** (2024), "Deciphering the Internal Conversion Processes Involved in Photochemical Ring-Opening of 1,3-Cyclohexadiene by Symmetric $sp^2$-Carbon Substitutions", J. Phys. Chem. A **128**, 2025 – 2037 (**This article has appeared as a Cover Feature of the Journal**).

29. N. Keot and **M. Sarma*** (2023), "Probing the Dynamic Behaviour and Magnetic Identification of Seven Coordinated Mn(II) Complexes: A Combined AIMD and Multireference Approach", Phys. Chem. Chem. Phys. **25**, 31165 – 31177.

30. N. Keot, B. Lama, H. K. Singh, H. P. Bhattacharyya, and **M. Sarma*** (2023), "Unveiling the Noncovalent Interaction of Thiazol-2-ylidene and its Derivatives as N-heterocyclic Carbene with Different Proton Donor Molecules", ChemPhysChem **24**, e202300413 (1 – 11).

31. H. K. Singh, U. Nath, N. Keot, and **M. Sarma*** (2023), "Exploring π-π Interactions and Electron Transport in Complexes Involving Hexacationic Host and PAH Guest: A Promising Avenue for Molecular Devices", Phys. Chem. Chem. Phys. **25**, 26767 – 26778.

32. **A. Sarmah***, M. Sarma, **M. Sarma**, and P. Hobza (2023), "Functional Design of a Reconfigurable Molecular Nanomachine: A Promising Domain for Optically Propelled Molecular Motors", J. Phys. Chem. C **127**, 18574 – 18585.

33. T. L. Fischer, M. Bödecker, S. M. Schweer, J. Dupont, V. Lepère, A. Zehnacker-Rentien, M. A. Suhm, B. Schröder, T. Henkes, D. M. Andrada, R. M. Balabin, H. K. Singh, H. P. Bhattacharyya, **M. Sarma**, S. Käser, K. Töpfer, L. I. Vazquez-Salazar, E. D. Boittier, M. Meuwly, G. Mandelli, C. Lanzi, R. Conte, M. Ceotto, F. Dietrich, V. Cisternas, R. Gnanasekaran, M. Hippler, M. Jarraya, M. Hochlaf, N. Viswanathan, T. Nevolianis, G. Rath, W. A. Kopp, K. Leonhard, and **R. A. Mata*** (2023), "The First HyDRA Challenge for Computational Vibrational Spectroscopy", Phys. Chem. Chem. Phys. **25**, 22089 – 22102.

34. S. Kumar, H. K. Singh, H. P. Bhattacharyya, and **M. Sarma*** (2023), "Low Energy Electron Interaction with Citric Acid: A Local Complex Potential based Time-Dependent Wavepacket Study", J. Chem. Sci. **135**, 88 (1 – 10). (invited contribution

in the Special Issue on Interplay of Structure and Dynamics in Reaction Pathways, Chemical Reactivity and Biological Systems)

35. R. Saini, G. R. Navale, S. Singh, H. K. Singh, R. Chauhan, S. Agrawal, D. Sarkar, **M. Sarma**, and **K. Ghosh*** (2023), "Inhibition of amyloid $\beta_{1\text{-}42}$ Peptide Aggregation by Newly Designed Cyclometallated Palladium Complexes", Int. J. Biol. Macromol. **248**, 125847 (1 – 13).

36. Md. T. Hossain, L. P. L. Mawlong, T. Jena, A. Bora, U. Nath, **M. Sarma**, and **P. K. Giri*** (2023), "Interlayer Charge-Transfer-Induced Photoluminescence Quenching and Enhanced Photoconduction in Two-Dimensional $Bi_2O_2Se/MoS_2$ Type-II Heterojunction", ACS Appl. Nano Mater. **6**, 11023 – 11036.

37. Md. T. Hossain, T. Jena, U. Nath, **M. Sarma**, and **P. K. Giri*** (2023), "Room Temperature Exciton Formation and Robust Optical Properties of CVD-Grown Ultrathin $Bi_2O_2Se$ Crystals on Arbitrary Substrates", Nanoscale **15**, 11222 – 11236.

38. H. K. Singh, R. R. Changmai, N. Keot, H. P. Bhattacharyya, and **M. Sarma*** (2023), "A Computational Insight on the Noncovalent Interactions of Aminothiazole-based Palladium(II) Complexes with DNA as a Potent Anticancer Agent", Polyhedron **239**, 116448 (1 – 12).

39. S. Singh, G. R. Navale, S. Agrawal, H. K. Singh, L. Singla, D. Sarkar, **M. Sarma**, A. Roy Choudhury, and **K. Ghosh*** (2023), "Design and Synthesis of Piano-Stool Ruthenium(II) Complexes and their Studies on the Inhibition of amyloid β (1-42) Peptide Aggregation", Int. J. Biol. Macromol. **239**, 124197 (1 – 17).

40. H. K. Singh and **M. Sarma*** (2023), "Torsional Rotation in Ditopic Receptor Host and its Complex Formation with Resorcinol Guest: A Computational Study", ChemPhysChem **24**, e202200928 (1 – 12).

41. U. Nath and **M. Sarma*** (2023), "Pyridinic Dominance N-Doped Graphene: A Potential Material for $SO_2$ Gas Detection", J. Phys. Chem. A **127**, 1112 – 1123.

42. T. Jena, Md. T. Hossain, U. Nath, **M. Sarma**, H. Sugimoto, M. Fujii, and **P. K. Giri*** (2023), "Evidence for Intrinsic Defects and Nanopores as Hotspots in 2D $PdSe_2$ Dendrites for Plasmon-free SERS Substrate with a High Enhancement Factor", npj 2D Mater Appl **7**, 8 (1 – 13).

43. P. Kalita[#], B. Medhi[#], H. K. Singh, H. P. Bhattacharyya, N. Gupt, and **M. Sarma*** (2023), "Perturbing π-clouds with Substituents to Study the Effects on Reaction Dynamics of gauche-1,3-Butadiene to Bicyclobutane Electrocyclization", ChemPhysChem **24**, e202200727 (1 – 9). (invited contribution in the Special Collection of Theoretical Chemistry Symposium 2021) [# Equal Contribution]

44. N. Keot and **M. Sarma*** (2023), "Computational Insight into a Mechanistic Overview of Water-Exchange Kinetics and Thermodynamic Stabilities of Bis and Tris-Aquated Complexes of Lanthanides", RSC Adv. **13**, 1516 – 1529.

45. B. Lama and **M. Sarma*** (2022), "Unraveling the Mechanistic Pathway for the Dual Fluorescence in Green Fluorescent Protein (GFP) Chromophore Analogue: A Detailed Theoretical Investigation", J. Phys. Chem. B **126**, 9930 – 9944 (**This article has appeared as a Cover Feature of the Journal**).

46. R. R. Changmai and **M. Sarma*** (2022), "Tropospheric Oxidation of Dichlorotetrafluoropropene ($CF_3$-$CF$=$CCl_2$) Initiated by OH Radical: Reaction Mechanisms, Kinetic Studies, and Atmospheric Implications", ACS Earth Space Chem. **6**, 1782 – 1792.

47. B. K. Rajbongshi*, H. P. Bhattacharyya[#], C. D. Pegu[#], S. Sharma, P. K. Baruah*, and **M. Sarma*** (2022), "Ultra-High Stokes Shift in Polycyclic Chromeno [2,3-*b*] Indoles", Polycycl. Aromat. Comp. **42**, 1710 – 1727. [# Equal Contribution]

48. S. B. Sarmah, P. Kalita*, B. Das, A. Garg, L. Gao, R. K. Pai, and **M. Sarma** (2020), "Numerical and Experimental Investigation of State of Health of Li-ion Battery", Int. J. Green Energy **17**, 510 – 520.

49. A. Rana and **M. Sarma*** (2019), "Computational Investigation of Dissociative Electron Attachment to Ammonia", J. Indian Chem. Soc. **96**, 785 – 791. (invited contribution in the Special Issue of Theoretical Chemistry)

50. A. Buragohain, M. Yousufuddin, **M. Sarma**, and S. Biswas* (2016), "3D Luminescent Amide-Functionalized Cadmium Tetrazolate Framework for Selective Detection of 2, 4, 6 – Trinitrophenol", Cryst. Growth Des. **16**, 842 – 851.

51. R. Bhaskaran and **M. Sarma*** (2015), "Low-Energy Electron Interaction with the Phosphate Group in DNA Molecule and the Characteristics of Single-Strand Break Pathways", J. Phys. Chem. A **119**, 10130 – 10136.

52. R. Bhaskaran and **M. Sarma*** (2015), "The Role of the Shape Resonance State in Low Energy Electron Induced Single Strand Break in 2′-deoxycytidine-5′-monophosphate", Phys. Chem. Chem. Phys. **17**, 15250 – 15257.

53. R. Bhaskaran and **M. Sarma*** (2014), "Low Energy Electron Induced Cytosine Base Release in 2′-deoxycytidine-3′-monophosphate Via Glycosidic Bond Cleavage : A Time-Dependent Wave Packet Study", J. Chem. Phys. **141**, 104309 (1 – 9).

54. R. Bhaskaran and **M. Sarma*** (2013), "Effect of Quantum Tunneling on Single Strand Breaks in a Modeled Gas Phase Cytidine Nucleotide Induced by Low Energy Electron: A Theoretical Approach", J. Chem. Phys. **139**, 045103 (1 – 9).

55. B. K. Shandilya, **M. Sarma***, S. Adhikari*, and M. K. Mishra (2013), "Time Dependent Wave Packet Treatment of $^2\Pi_g$ $N_2^-$ and $^3\Sigma^-$ $NO^-$ Shape Resonances Using Two-Dimensional Surfaces for Electron – $N_2$ and NO Interactions", Int. J. Quantum Chem. **113**, 130 – 138.

56. S. Bhowmick, Renjith B., M. K. Mishra, and **M. Sarma*** (2012), "Investigation of Dissociative Electron Attachment to 2′-deoxycytidine-3′-monophosphate Using DFT Method and Time Dependent Wave Packet Approach", J. Chem. Phys. **137,** 064310 (1 – 8).

57. B. K. Shandilya, **M. Sarma***, S. Adhikari, and M. K. Mishra (2012), "Vibrational Excitation Resulting from Electron Capture in LUMO of $F_2$ and HCl – A Treatment Using the Time-Dependent Wave Packet Approach", J. Chem. Sci. **124**, 141 – 148. (invited contribution)

58. Renjith B., S. Bhowmick, M. K. Mishra, and **M. Sarma*** (2011) "Low-Energy Electron-Induced Single Strand Breaks in 2′-deoxycytidine-3′-monophosphate Using the Local Complex Potential Based Time-Dependent Wave Packet Approach", J. Phys. Chem. A **115,** 13753 – 13758.

59. **M. Sarma*** and **M. K. Mishra*** (2009), "Treatment of Vibrational Fine Structure in Resonant e-Diatom Scattering using Local Complex Potentials (LCPs) and Time Dependent Wave Packet (TDWP) Approach", Adv. Quantum Chem. (invited review, in press)

60. **M. Sarma**, S. Adhikari, and M. K. Mishra* (2009), "Laser Assisted Control of Selective Bond Dissociation in HOD – Some Mechanistic Insights", Mol. Phys. **107**, 939 – 961.

61. **M. Sarma**, S. Adhikari, and M. K. Mishra* (2008), "An Examination of the Expectation Value Profiles for Average Stretch and Momentum in O–H and O–D Bonds of the HOD Molecule To Determine Their Role in Selective Photodissociation", J. Phys. Chem. A **112**, 13302 – 13307.

62. **M. Sarma** and M. K. Mishra* (2008), "Role of Photolysis Frequency in Enhanced Selectivity and Yield for Controlled Bond Breaking in HOD", J. Phys. Chem. A **112**, 4895 – 4905.

63. **M. Sarma**, S. Adhikari, and M. K. Mishra (2008), "Mechanistic Investigation of Vibrational Fine Structure in e – $H_2$ Scattering Using Local Complex Potential-Based Time Dependent Wave Packet Approach", Int. J. Quantum Chem. **108**, 1044 – 1051.

64. R. K. Singh, **M. Sarma**, and M. K. Mishra* (2007), "Approximate Construction of Local Complex Potentials for a Time Dependent Wave Packet based Treatment of Vibrational Excitation Cross-sections in Resonant e – $N_2$, e – CO and e – $H_2$ Scattering", Indian J. Phys. **81**, 983 – 1002. (invited contribution)

65. R. K. Singh, **M. Sarma**, A. Jain, S. Adhikari, and M. K. Mishra* (2007), "Calculation of Vibrational Excitation Cross-sections in Resonant Electron-Molecule Scattering Using the Time-Dependent Wave Packet Approach with

Application to the $^2\Pi$ $CO^-$ Shape Resonance", J. Chem. Sci. **119**, 385 – 389. (invited contribution)

66. **M. Sarma**, S. Adhikari, and M. K. Mishra* (2007), "Selective Control of HOD Photodissociation Using CW Lasers", J. Chem. Sci. **119**, 377 – 384. (invited contribution)

67. **M. Sarma**, S. Adhikari, and M. K. Mishra* (2007), "Selective Photodissociation of O–H and O–D Bonds from Ground Vibrational State of HOD Using Simple UV Pulses", J. Chem. Phys. **127**, 024305 (1 – 5).

68. **M. Sarma**, S. Adhikari, and M. K. Mishra* (2007), "Simple Systematization of Vibrational Excitation Cross-section Calculations for Resonant Electron-Molecule Scattering in the Boomerang and Impulse Models", J. Chem. Phys. **126**, 044309 (1 – 5).

69. S. Adhikari, S. Deshpande, **M. Sarma**, V. Kurkal, and M. K. Mishra* (2006), "Selective Control of Photodissociation in Deutereted Water Molecule HOD", Radiat. Phys. Chem. **75**, 2106 – 2118.

70. **M. Sarma**, S. Adhikari, and M. K. Mishra* (2006), "Selective Control of HOD Photodissociation Using Low Quanta O–D Excitation and Field Optimized Initial State (FOIST) based Combination of States and Colors", Chem. Phys. Lett. **420**, 321 – 329.

**Research Publications in Books, Book Chapters, Book Series** [* Corresponding Author]

1. R. Chyrmang, U. Nath, and **M. Sarma*** (2024), "Insight into the Structural, Electronic, and Magnetic Properties of Mn, Fe, and Co-doped Bilayer Borophene", in Theoretical Methods, Algorithms and Applications of Quantum Systems in Chemistry, Physics and Biology, Progress in Theoretical Chemistry and Physics, Springer (in press).

2. B. K. Shandilya, **M. Sarma***, S. Adhikari, and M K Mishra* (2015), "Selective Photodissociation of Bonds in $^{18}O^{16}O^{16}O$ Molecule", in Advances in Laser Physics and Technology, Ed. Man Mohan, Cambridge University Press, pp. 54 – 69.

3. B. K. Shandilya, **M. Sarma***, V. Kurkal-Siebert, S. Adhikari, and M. K. Mishra* (2013), "Selective Photodynamic Control of Bond Dissociation Using Optimal Initial Vibtrational States", in Concepts and Methods in Modern Theoretical Chemistry: Statistical Mechanics, Eds. P. K. Chattaraj and S. K. Ghosh, Taylor & Francis / CRC Press, pp. 113 – 162.

4. **M. Sarma**, S. Adhikari, S. Deshpande, Vandana K., and M. K. Mishra* (2008), "Selective Control of Photodissociation in HOD", in Atoms and Molecules in Laser and External Fields, Ed. Man Mohan, Narosa Publications, pp. 59 – 70.

**Research Publications in Conference Proceedings** [* Corresponding Author]

1. **R. Chyrmang,** U. Nath, and M. Sarma*, "*Detection of 5-methylcytosine and 5-hydroxymethylcytosine on the Hydrogenated Borophene Nanochannel*", Society of Physical Chemistry Symposium – 2025 (SoPhyC-2025), October 11 – 14, 2025, Indian Institute of Technology (IIT) Patna, Patna, India (Poster).

2. **A. K. Yadav,** R. R. Changmai, S. R. Daimari, and M. Sarma*, "*Theoretical Kinetic Modelling of the Reaction between n-propanol and $NH_2$ Radical in the Interstellar Medium*", Society of Physical Chemistry Symposium – 2025 (SoPhyC-2025), October 11 – 14, 2025, Indian Institute of Technology (IIT) Patna, Patna, India (Poster).

3. **M. P. Sarmah,** B. Medhi, and M. Sarma*****, "*Mechanistic Insight into the Electron Attachment on Dipeptides*", 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC) 2025, June 22 – 27, 2025, Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo, Oslo, Norway (Poster).

4. S. Kumar and **M. Sarma***, "*Low Energy Electron Induced DNA Damage: A Theoretical Viewpoint*", Chem Convergence 2025: Advancing Chemistry Through Multidisciplinary Innovations, March 04 – 07, 2025, Madanapalle Institute of Technology & Science, Madanapalle, Andhra Pradesh, India (Plenary Talk).

5. N. Keot and **M. Sarma***, "*Computational Study of Transition Metal and Lanthanide Complexes: From Imaging to Magnetism*", International Conference on Frontiers in Chemical Sciences – 2025 (ICFCS-2025), March 01 – 03, 2025, Central University of Jharkhand, Ranchi, Jharkhand, India (Plenary Talk).

6. **M. P. Sarmah**, B. Medhi and M. Sarma*, "*Impact on the Electron Attachment to the Alanylglycine and GlycylAlanine*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2025, February 20 – 23, 2025, Mussoorie, Uttarakhand, India (Poster).

7. **S. Kumar** and M. Sarma*, "*Study of Electron Capture by 5-halogenated Cytosine in Gas and Aqueous Phases*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2025, February 20 – 23, 2025, Mussoorie, Uttarakhand, India (Poster).

8. B. Medhi and **M. Sarma***, "*Mechanistic Exploration of Photochemical Ring Opening and Closure in Conjugated Polyenes*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2025, February 20 – 23, 2025, Mussoorie, Uttarakhand, India (Invited Talk).

9. **R. R. Changmai** and M. Sarma*, "*Theoretical Study of the Mechanism, Thermodynamics and Kinetics of the Reaction of $CF_3CH_2CFCl_2$ (HCFC-234fb) with OH-radicals and Cl-atoms*", Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems – 2024 (PCAMC-2024), December 11 – 14, 2024, Indian

Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

10. **U. Nath** and M. Sarma*, "*Charge-controlled $CO_2$ Activation and Electrochemical Reduction on Free-standing Defect-induced Bilayer Borophene*", Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems – 2024 (PCAMC-2024), December 11 – 14, 2024, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

11. B. Lama and **M. Sarma***, "*Insights into Photodynamics Simulation of Excited-State Relaxation Mechanism of GFP Chromophore and its Derivatives*", Physics and Chemistry of Atomic, Molecular and Condensed Matter Systems – 2024 (PCAMC-2024), December 11 – 14, 2024, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Invited Talk).

12. **H. P. Bhattacharyya** and M. Sarma*, "*Maximum Efficiency of Catalysts: A Theoretical Investigation Through MaxKinEff Model*", Physical Chemistry Symposium – 2024 (SoPhyC-2024), October 22 – 25, 2024, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Poster).

13. **J. Dutta** and M. Sarma*, "*Role of Noncovalent Interactions in Designing Selenium-based Antidepressants*", Physical Chemistry Symposium – 2024 (SoPhyC-2024), October 22 – 25, 2024, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Poster).

14. H. P. Bhattacharyya and **M. Sarma***, "*Efficiency Conceptualization Model for Unveiling the Efficiency of Catalysts*", Physical Chemistry Symposium – 2024 (SoPhyC-2024), October 22 – 25, 2024, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Invited Talk).

15. **S. R. Daimari**, R. R. Changmai, and M. Sarma*, "*Theoretical Study of Hydroxyl Radical Initiated Oxidation Reaction for a Series of Expoxybutane Isomers*", Current Trends in Theoretical Chemistry – 2024 (CTTC–2024), September 26 – 28, 2024, Bhabha Atomic Research Centre, Mumbai, India (Poster).

16. **B. Medhi** and M. Sarma*, "*Exploring Fulgide Photochromism: Mechanistic Pathways and Electron Transport via Computational Approach*", CZS Summer School 2024 on "Machine Learning for Chemistry", September 09 – 13, 2024, Triangel Workspace, Karlsruhe, Germany (Poster).

17. **B. Lama** and M. Sarma*****, "*Hot Excitonic Behavior in a GFP Chromophore Derivative via Excited-State Nonadiabatic Dynamics*", 29$^{th}$ IUPAC Symposium on Photochemistry (29$^{th}$ PhotoIUPAC), July 14 – 19, 2024, Valencia Conference Centre, Valencia, Spain (Poster).

18. S. R. Daimari, R. R. Changmai, and **M. Sarma***, "*A Theoretical Perspective on OH Radical-Initiated Oxidation Reactions of Epoxybutane Isomers*", 2nd National Conference on Emerging Challenges in the Frontiers of Chemical Sciences

(NC-ECFCS-2024), March 21 – 13, 2024, Department of Chemistry, Manipur University, Manipur, India (Invited Talk).

19. **S. R. Daimari**, R. R. Changmai, and M. Sarma*****, "*Hydroxyl Radical Initiated Oxidation Reaction for a Series of Expoxybutane Isomers: A Theoretical Perspective*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

20. **M. P. Sarmah** and M. Sarma*****, "*Effect of Arginine in the Electron Attachment to Guanosine*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

21. **S. Kumar** and M. Sarma*****, "*Unraveling the Impact of Dissociative Electron Attachment on Halogenated 2′-deoxycytidine-3′-monophosphate*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

22. **R. R. Changmai**, S. R. Daimari, and M. Sarma*****, "*Tropospheric Oxidation of HCFC-234fb initiated by •OH-radical and Cl-atom*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

23. **B. Medhi** and M. Sarma*****, "*Unraveling Fulgide Photochromism: A Computational Approach to Mechanistic Understanding*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

24. **M. Sarma** and M. Sarma*****, "*A Computational Study on the Binding Affinity of Tetrahedral Anions to the Polyglycine Receptor*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

25. **U. Nath** and M. Sarma*****, "*Two-dimensional Oxygen Functionalized Boron Sulfide (Oh-$B_2S_2$) Monolayer: An Effective Nanosensor for NO and $NO_2$ Detection*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

26. **N. Keot** and M. Sarma*****, "*Solution dynamics and Magnetic Properties of Seven-Coordinate Mn(II) Complexes: Implications for Magnetic Resonance Imaging and Single Molecule Magnets*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (Poster).

27. **H. P. Bhattacharyya** and M. Sarma*, "*Efficiency Conceptualization Model in the light of Bio-Inspired Molecular Water Oxidation Catalysts*", 6th Symposium on Advanced Biological Inorganic Chemistry (SABIC) 2024, January 07 – 11, 2024, Indian Association for the Cultivation of Science (IACS), Kolkata, India (Poster).

28. **M. P. Sarmah** and M. Sarma*, "*Impact of Electron Attachment to Guanosine in the Presence of Amino Acid*", 17th DAE-BRNS Biennial Trombay Symposium on Radiation & Photochemistry (TSRP-2024), January 07 – 11, 2024, Bhabha Atomic Research Centre, Mumbai, India (Poster).

29. **S. Kumar** and M. Sarma*****, "*Investigation of Dissociative Electron Attachment to Halogenated 2´-deoxycytidine-3´-monophosphate*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

30. **R. R. Changmai** and M. Sarma*****, "*Atmospheric Oxidation of HCFC-234fb initiated by •OH-Radical and Cl-atom*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

31. **B. Medhi** and M. Sarma*****, "*Decoding Fulgide Photochromism: Computational Perspectives on Mechanistic Understanding*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

32. **M. Sarma** and M. Sarma*****, "*Investigating the Dynamic and Electronic Properties of Oligo-Glycine as a Tetrahedral Anion Receptor*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

33. **U. Nath** and M. Sarma*****, "*Insight into the Surface Oxygen Functionalized $B_2S_2$ Monolayer for NO and $NO_2$ Detection*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

34. **N. Keot** and M. Sarma*****, "*Dynamic Properties and Magnetic Characterization of Seven-Coordinate Mn(II) Complexes for their Application in Magnetic Resonance Imaging and Single Molecule Magnets*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

35. **B. Lama** and M. Sarma*****, "*Hot Exciton Behavior in Green Fluorescent Protein (GFP) Chromophore Analogue via Nonadiabatic Dynamics*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Poster).

36. N. Keot and **M. Sarma***, "*Role of Lanthanide Based Complexes and Transition Metals in Magnetic Resonance Imaging (MRI) and Single Molecule Magnets (SMMs)*", Theoretical Chemistry Symposium (TCS) 2023, December 07 – 10, 2023, Indian Institute of Technology (IIT) Madras, Chennai, India (Invited Talk).

37. U. Nath and **M. Sarma***, "*Chemical Sensing via Atomically Modified 2D Materials*", 26th International Workshop on Quantum Systems in Chemistry, Physics, and

Biology (QSCP-XXVI), October 14 – 20, 2023, Jaipur, Rajasthan, India (Invited Talk).

38. **S. Kumar** and M. Sarma*, "*Low-Energy Electron Attachment to Citric Acid: A Mixed Electronic Structure and Quantum Dynamics Study*", 6th International Conference on Molecular Simulation (ICMS 2023), October 06 – 09, 2023, National Taiwan University, Taipei, Taiwan (Poster).

39. **H. P. Bhattacharyya** and M. Sarma*, "*Developing a Model to Theoretically Assess the Turnover Frequency in the Light of Collision Theory*", 6th International Conference on Molecular Simulation (ICMS 2023), October 06 – 09, 2023, National Taiwan University, Taipei, Taiwan (Oral Talk).

40. **U. Nath** and M. Sarma*, "*First Principle Investigation of Pyridinic N-doped Graphene as a Potential $SO_2$ Gas Sensor*", Graphene 2023, June 27 – 30, 2023, The University of Manchester, Manchester, United Kingdom (Poster).

41. **H. K. Singh** and M. Sarma*, "*A Molecular Dynamics Perspective on Interaction between Amino Acid functionalized Perylenediimide and Amyloid-β fibrils*", Frontiers in Chemical Sciences (FICS) 2022, December 02 – 04, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

42. **R. R. Changmai** and M. Sarma*, "*Tropospheric Oxidation of CFC-alternatives Initiated by OH-Radical: A Computational Perspective*", Frontiers in Chemical Sciences (FICS) 2022, December 02 – 04, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

43. P. Kalita, **B. Medhi**, H. K. Singh, H. P. Bhattacharyya, N. Gupt, and M. Sarma*, "*Probing the Effects of Electron Withdrawing and Donating Substituents in gauche-1,3-Butadiene to Bicyclobutane Electrocyclization*", Recent Advances in Chemistry: Theoretical and Computational Aspects (RAC:TCA) 2022, November 18 – 20, 2022, National Institute of Technology (NIT) Meghalaya, Shillong, India (Poster).

44. **U. Nath** and M. Sarma*, "*Temperature-Dependent NO Adsorption and Desorption in N-doped Graphene Monolayer*", Recent Advances in Chemistry: Theoretical and Computational Aspects (RAC:TCA) 2022, November 18 – 20, 2022, National Institute of Technology (NIT) Meghalaya, Shillong, India (Poster).

45. U. Nath and **M. Sarma***, "*Pyridinic Nitrogen-Doped Graphene as an Efficient Sensor for $SO_2$ Detection: A Computational Perspective*", Recent Advances in Chemistry: Theoretical and Computational Aspects (RAC:TCA) 2022, November 18 – 20, 2022, National Institute of Technology Meghalaya (NIT), Shillong, India (Invited Talk).

46. **M. Sarma** and M. Sarma*, "*Molecular Recognition of Arsenite Towards Peptide Receptor: A Theoretical Investigation*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2022, November 10 – 13, 2022, Malpe, Karnataka, India (Poster).

47. **N. Keot** and M. Sarma*, "*Computational Evaluation of Structural, Bonding and Water Exchange Kinetics of Bis and Tris-aquated Complexes of Lanthanides*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2022, November 10 – 13, 2022, Malpe, Karnataka, India (Poster).

48. **R. R. Changmai** and M. Sarma*, "*Theoretical Studies on the Kinetics, Mechanism and Atmospheric Implications of the Gas-Phase Reaction of Dichlorotetrafluoropropene ($CF_3CF=CCl_2$) Initiated by OH radical*", Current Trends in Theoretical Chemistry – 2022 (CTTC-2022), September 22 – 24, 2022, Bhabha Atomic Research Centre, Mumbai, India (Poster).

49. **U. Nath** and M. Sarma*, "*Computational Investigation of Pyridinic Dominance Graphene as Sensor for Oxide-Containing Triatomic Gas Molecules*", Current Trends in Theoretical Chemistry – 2022 (CTTC-2022), September 22 – 24, 2022, Bhabha Atomic Research Centre, Mumbai, India (Poster).

50. **B. Lama** and M. Sarma*, "*Ultrafast Excited-State Intermolecular and Intermolecular Proton Transfer (ESIPT) Mechanism in Sulfonamide Analogues of GFP: A Theoretical Investigation*", Current Trends in Theoretical Chemistry – 2022 (CTTC-2022), September 22 – 24, 2022, Bhabha Atomic Research Centre, Mumbai, India (Poster).

51. **M. Sarma***, "*Excited-State Structural Events on the Dual Emissive Behavior of Green Fluorescent Protein (GFP) Chromophore Analogue: A Theoretical Investigation*", Current Trends in Theoretical Chemistry – 2022 (CTTC-2022), September 22 – 24, 2022, Bhabha Atomic Research Centre, Mumbai, India (Invited Talk).

52. H. K. Singh, H. P. Bhattacharyya, B. Lama, N. Keot, U. Nath, M. Sarma, B. Medhi, R. R. Changmai, and **M. Sarma***, "*Computational Exploration of Anti-Influenza Drugs as the Potential Inhibitor of SARS-CoV-2 $M^{pro}$: A Combined Docking and Molecular Dynamics Simulations Study*", The International Society of Quantum Biology and Pharmacology (ISQBP) 2022 President's Meeting, July 11 – 14, 2022, Offline and Online Meeting, Innsbruck, Austria (Poster).

53. **M. Sarma***, "*Effect of Electron Withdrawing and Electron Donating Groups in the Investigation of Dissociative Electron Attachment Cross – Section to Some Biomolecules*", 12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC) 2020, July 03 – 08, 2022, The University of British Columbia, Vancouver, Canada (Invited Talk).

54. H. P. Bhattacharyya and **M. Sarma***, "*Developing a Strategy for Predicting "Turning Over" of Catalysts: An ab initio Insights with Mononuclear Ruthenium-Catalyzed Water Oxidation Reaction*", Theoretical Chemistry Meeting: Structure and Dynamics-2022 (TCMSD-2022), May 26 – 29, 2022, Indian Association for the Cultivation of Science (IACS), Kolkata, India (Invited Talk).

55. **R. R. Changmai** and M. Sarma*, "*Atmospheric Degradation of CFC-Alternatives Initiated by OH-Radical: A Computational Study of the Reaction Mechanisms, Kinetic Studies, and Atmospheric Implications*", North-East Research Conclave, May 20 – 22, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

56. **B. Medhi** and M. Sarma*, "*Effects of Substitution on Reaction Dynamics at the Conical Intersections of Cyclohexadiene Molecule*", North-East Research Conclave, May 20 – 22, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

57. **M. Sarma** and M. Sarma*, "*Binding Affinity of Arsenite towards Amide Based Systems: A Theoretical Investigation*", North-East Research Conclave, May 20 – 22, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

58. **U. Nath** and M. Sarma*, "*Pyridinic Dominance Graphene as an Efficient and Selective Gas-Sensor Toward $SO_2$ Detection*", North-East Research Conclave, May 20 – 22, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

59. **N. Keot** and M. Sarma*, "*Understanding the Structural Properties and Water Exchange Rate of two Bis and Tris-aquated Complexes of Lanthanide: A Computational Study*", North-East Research Conclave, May 20 – 22, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

60. **H. P. Bhattacharyya** and M. Sarma*, "*Assessing the Efficiency for Water Splitting Reaction: A Step Towards Sustainable Development*", North-East Research Conclave, May 20 – 22, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Oral Talk).

61. H. K. Singh and **M. Sarma***, "*Computational Exploration of Noncovalent Interactions: From Supramolecular Host-Guest Complexes to Protein-Ligand Systems*", Advances in Sustainable Chemistry and Material Science-2022 (ASCMS-2022), April 29 – 30, 2022, Bodoland University, Kokrajhar, India (Invited Talk).

62. **R. R. Changmai** and M. Sarma*, "*Atmospheric Chemistry of Chlorofluorocarbon with Hydroxyl Radical: A Computational Investigation*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

63. **B. Medhi** and M. Sarma*, "*Effects of Substitution on Reaction Dynamics at the Conical Intersections of Cyclohexadiene Molecule*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

64. **M. Sarma** and M. Sarma*, "*Structural and Conformational Correlation for Tetra-peptide Chain of Glycine: A Theoretical Investigation*", Theoretical Chemistry

Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

65. **U. Nath** and M. Sarma*, "*Role of Vacancy on Electronic and Magnetic Properties of Pyridinic N-doped Graphene*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

66. **N. Keot** and M. Sarma*, "*Computational Investigation on Water Exchange Rates and Stability of Lanthanide-based MRI Contrasting Agent*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

67. **B. Lama** and M. Sarma*, "*Theoretical and Computational Investigation on Dual Fluorescence Mechanism of Green Fluorescent Protein (GFP)-like Chromophore*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

68. **H. P. Bhattacharyya** and M. Sarma*, "*Assessing the Efficiency with ECM Strategy: A Case Study to Artificial Water Splitting Reaction*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

69. **H. K. Singh** and M. Sarma*, "*Computational Investigation on the Nature of Host-Guest Interactions in PAHs-Hexacationic Cage Complexes*", Theoretical Chemistry Symposium (TCS) 2021, December 11 – 14, 2021, Online, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

70. **H. P. Bhattacharyya** and M. Sarma*, "*Roadmap for Designing the Strategy to Mimic the Experimental Turnover Numbers: A Case Study to Artificial Water Splitting Reaction*", 57th Symposium on Theoretical Chemistry, September 20 – 24, 2021, Online, University of Würzburg, Germany (Poster).

71. **H. K. Singh** and M. Sarma*, "*Computational Investigation of the Noncovalent Interactions in Ditopic Receptor Host and its Complex Formation with a Benzene Metabolite Resorcinol Molecule*", 57th Symposium on Theoretical Chemistry, September 20 – 24, 2021, Online, University of Würzburg, Germany (Poster).

72. **M. Sarma***, "*Effect of Resonance Width in the Investigation of Dissociative Electron Attachment Cross – Section to Some Bio Molecules*", The International Society of Quantum Biology and Pharmacology (ISQBP) 2021 President's Meeting, June 29 – July 01, 2021, Online Meeting, Strasbourg, France (Poster).

73. **U. Nath** and M. Sarma*, "*Adsorption of Individual CO Gas Molecule on Graphene: A Computational Investigation*", 57$^{th}$ Annual Convention of Chemists, 2020 & International Conference on Recent Trends in Chemical Sciences (RTCS) 2020, December 26 – 29, 2020, Online, India (Poster).

74. **N. Keot** and M. Sarma*, "*Computational Investigation on Water Exchange Rates of different Stereo-isomers of Lanthanides Complexes*", 57th Annual Convention of Chemists, 2020 & International Conference on Recent Trends in Chemical Sciences (RTCS) 2020, December 26 – 29, 2020, Online, India (Poster).

75. **B. Lama** and M. Sarma*, "*Theoretical and Computational Investigation of the Excited State Dynamics of the Green Fluorescent Protein and its Variants*", 57th Annual Convention of Chemists, 2020 & International Conference on Recent Trends in Chemical Sciences (RTCS) 2020, December 26 – 29, 2020, Online, India (Poster).

76. **H. P. Bhattacharyya** and M. Sarma*, "*Molecular Water Oxidation Catalyst(s): An Approach for Predicting the Efficiency*", 57th Annual Convention of Chemists, 2020 & International Conference on Recent Trends in Chemical Sciences (RTCS) 2020, December 26 – 29, 2020, Online, India (Oral Talk).

77. **M. Sarma***, "*Density Functional Theory in Electron-Molecule Scattering with an Application to Biomolecules*", New Horizons in Density Functional Theory Faraday Discussion, September 02 – 04, 2020, Online, United Kingdom (Poster).

78. **K. Talukdar** and M. Sarma*, "*Determination of Vertical Attachment Energy of 2′-deoxy Adenosine-3′-Monophosphate using Restricted and Unrestricted Hartree-Fock Method with the 6-31+G(d) as the Basis Set*", International e – Poster Conference on Current Outlook in Material Science and Engineering 2020 (COMSE – 2k20), May 15 – 16, 2020, Facebook, India (Poster). [Organizer(s): Bodoland University, Tripura University, ADP College, Nagaon and MIT Aurangabad]

79. **H. P. Bhattacharyya** and M. Sarma*, "*Prediction of Efficiency of Photocatalyst(s) in Water Splitting: A Computational Study*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2020, February 20 – 23, 2020, Kumbhalgarh, Rajasthan, India (Poster).

80. **H. K. Singh** and M. Sarma*, "*Analysing the Noncovalent Interactions between the Ditopic Receptor Host and Guest Benzene Metabolite Molecules through Density Functional Theory (DFT) Calculation*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2020, February 20 – 23, 2020, Kumbhalgarh, Rajasthan, India (Poster).

81. **M. Sarma***, "*Theoretical Chemistry: An Interplay between Structure and Dynamics*", Emerging Trends in Chemical Sciences (ETCS) 2020, February 13 – 15, 2020, Gauhati University, Guwahati, India (Invited Talk).

82. **H. P. Bhattacharyya** and M. Sarma*, "*Efficiency of a Photocatalyst: A Computational Investigation*", Recent Advances in Chemistry (RAC) 2019, October 14 – 15, 2019, National Institute of Technology (NIT) Meghalaya, Shillong, India (Poster).

83. **H. K. Singh** and M. Sarma*****, "*DFT Studies on the Interaction between the Ditopic Receptor and Benzene Metabolites*", Recent Advances in Chemistry (RAC) 2019, October 14 – 15, 2019, National Institute of Technology (NIT) Meghalaya, Shillong, India (Poster).

84. **M. Sarma***, "*Interplay between Structure and Dynamics*", Recent Advances in Chemistry (RAC) 2019, October 14 – 15, 2019, National Institute of Technology (NIT) Meghalaya, Shillong, India (Invited Talk).

85. H. P. Bhattacharyya and **M. Sarma***, "*Theoretical Investigation of Efficiency of a Photo Catalyst in Water Splitting*", Mechanistic Processes in Organometallic Chemistry Faraday Discussion, September 02 – 04, 2019, University of York, United Kingdom (Poster).

86. **H. K. Singh** and M. Sarma*****, "*Investigation of the Interaction of the Different Groups Modulated Galantamine Drug with Acetyl Cholinesterase by Molecular Docking and ONIOM Model*", Theoretical Chemistry Symposium (TCS) 2019, February 13 – 16, 2019, Birla Institute of Technology and Science (BITS), Pilani, India (Poster).

87. **M. Sarma***, "*Implementation of Local Complex Potential based Time Dependent Wave Approach in Electron Induced Chemistry*", Theoretical Chemistry Symposium (TCS) 2019, February 13 – 16, 2019, Birla Institute of Technology and Science (BITS), Pilani, India (Invited Talk).

88. R. Bhaskaran and **M. Sarma***, "*Investigation of Dissociative Electron Attachment Cross – Section to Some Biomolecules*", Gordon Research Conference on Computational Chemistry 2018, July 22 – 27, 2018, Mount Snow, West Dover, Vermont, United States of America (Poster).

89. **M. Sarma***, "*Resonances in Electron Molecule Scattering: Application to Some Bio Molecules*", National Conference on Applied Sciences, Sustainable and Evolving Technologies (ASSET) and 63$^{rd}$ Annual Technical Session of Assam Science Society, March 09 – 11, 2018, CIT Kokrajhar, Kokrajhar, India (Invited Talk).

90. **M. Sarma***, "*Local Complex Potential Based Time Dependent Wave Packet Approach in Electron Molecule Scattering*", IACS – Conference on Electronic Structure, Spectroscopy, and Dynamics (IACS – CESSD) 2018, February 22 – 25, 2018, Indian Association for the Cultivation of Science (IACS), Kolkata, India (Invited Talk).

91. R. Bhaskaran and **M. Sarma***, "*Low Energy Resonant Electron Scattering Off DNA Fragments*", Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2018, February 15 – 18, 2018, Dooars, Darjeeling, India (Invited Talk).

92. R. Bhaskaran and **M. Sarma***, "*Electron Induced Chemistry: Application to Some Bio Molecules*", MKM Mini Symposium, October 31, 2017, Department of Chemistry, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Invited Talk).

93. R. Bhaskaran and **M. Sarma***, "*Low Energy Electron Induced Damage to Selected DNA Fragments*", 4th International Conference on Physical and Theoretical Chemistry, September 18 – 19, 2017, Dublin, Ireland (Invited Talk).

94. **S. Goswami**, R. Bhaskaran and M. Sarma*, "*Effect of Substituents on Single Strand Breaks in a Selected DNA Fragment Induced by Low Energy Electrons*", CHEM CONVENE 17, July 25, 2017, Department of Chemistry, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

95. **M. Sarma***, "*Interplay between Structure and Dynamics*", CHEM CONVENE 17, July 25, 2017, Department of Chemistry, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Invited Talk).

96. R. Bhaskaran and **M. Sarma***, "*Low Energy Electron Induced Single Strand Breaks in Sugar-Phosphate-Sugar Fragment*", National Conference on Chemical Physics (NCCP) 2017, March 20 – 21, 2017, Assam University, Silchar, India (Invited Talk).

97. R. Bhaskaran and **M. Sarma***, "*Low Energy Electron Induced Single Strand Breaks in 2′-deoxy Cytidine-3′-Monophosphate*", Theoretical Chemistry Symposium (TCS) 2014, December 18 – 21, 2014, National Chemical Laboratory (CSIR-NCL), Pune, India (Invited Talk).

98. **Renjith B.**, S. Bhowmick, M. K. Mishra, and M. Sarma*, "*LEE Induced SSB in 2′-deoxy Cytidine-3′-Monophosphate Using LCP-TDWP Approach*", Theoretical Chemistry Symposium (TCS) 2012, December 19 – 22, 2012, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

99. **Renjith B.**, S. Bhowmick, M. K. Mishra, and M. Sarma*, "*Dissociative Electron Attachment to 2′-deoxy Cytidine-3′-Monophosphate*", National Symposium on Current Trends in Computational Chemistry (CTCC) 2012, March 16 – 17, 2012, North-Eastern Hill University (NEHU), Shillong, India (Poster).

100. **Renjith B.**, S. Bhowmick, M. K. Mishra, and M. Sarma*, "*Dissociative Electron Attachment to 2′-deoxy Cytidine-3′-Monophosphate*", 14th National Symposium in Chemistry (NSC – 14), February 03 – 05, 2012, Thiruvananthapuram, India (Poster).

101. **B. K. Shandilya**, M. Sarma, S. Adhikari, and M. K. Mishra*, "*Selective Control of Photodissociation in Isotopic Substituted Ozone ($^{18}O^{16}O^{16}O$) Molecule*", National Symposium on New Horizons in Chemistry, October 03 – 04, 2011, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Poster).

102. **B. K. Shandilya**, M. Sarma, S. Adhikari, and M. K. Mishra*, "*Selective Control of Photodissociation in Isotopic Substituted Ozone ($^{18}O^{16}O^{16}O$) Molecule*", Conference on Molecular Energy Transfer (COMET) 2011, September 11 – 16, 2011, University of Oxford, UK (Poster).

103. **B. K. Shandilya**, M. Sarma, S. Adhikari, and M. K. Mishra*, *"Vibrational Excitation Resulting from Electron Capture in LUMO of $F_2$, HCl – A Treatment Using the TDWP Approach"*, Theoretical Chemistry Symposium (TCS) 2010, December 08 – 12, 2010, Indian Institute of Technology (IIT) Kanpur, Kanpur, India (Poster).

104. M. Sarma, S. Adhikari, and **M. K. Mishra***, *"Some New Approaches to Photon Molecule Dynamics",* Theoretical Chemistry Symposium (TCS) 2010, December 08 – 12, 2010, Indian Institute of Technology (IIT) Kanpur, Kanpur, India (Invited Talk).

105. **Renjith B.**, S. Bhowmick, and M. Sarma*, "*Low Energy Electron Attachment to 2′-deoxy Cytidine Monophosphate*", Theoretical Chemistry Symposium (TCS) 2010, December 08 – 12, 2010, Indian Institute of Technology (IIT) Kanpur, Kanpur, India (Poster).

106. **B. K. Shandilya**, M. Sarma, S. Adhikari, and M. K. Mishra*, *"Vibrational Excitation Resulting from Electron Capture in LUMO of $F_2$, HCl – A Treatment Using the TDWP Approach",* Frontiers in Chemical Sciences (FICS) 2010, December 03 – 04, 2010, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

107. **Renjith B.**, **S. Bhowmick**, and M. Sarma*, "*Low Energy Electron Attachment to Cytidine Monophosphate*", Frontiers in Chemical Sciences (FICS) 2010, December 03 – 04, 2010, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Poster).

108. **B. K. Shandilya**, M. Sarma, S. Adhikari, and M. K. Mishra*, *"Treatment of $^2\Pi_g$ $N_2^-$ Shape Resonance using a Two Dimensional Surface and Time Dependent Wave Packet (TDWP) Approach",* International Conference and Humboldt Kolleg, February 24 – 27, 2010, University of Lucknow and Humboldt Academy Lucknow, Lucknow, India (Poster).

109. **M. Sarma**, S. Adhikari, and M. K. Mishra*, *"Selective Bond Cleavage in Unimolecular Reactions: A Detailed Investigation",* International Conference and Humboldt Kolleg, February 24 – 27, 2010, University of Lucknow and Humboldt Academy Lucknow, Lucknow, India (Invited Talk).

110. **B. K. Shandilya**, **M. Sarma**, S. Adhikari, and M. K. Mishra*, *"Treatment of $^2\Pi_g$ $N_2^-$ Shape Resonance using a Two Dimensional Surface and Time Dependent Wave Packet (TDWP) Approach",* Recent Advances in Many Electron Theories (RAMET) 2010, January 05 – 07, 2010, Shankarpur, India (Poster).

111. **B. K. Shandilya**, **M. Sarma**, S. Adhikari, and M. K. Mishra*, *"Treatment of $^2\Pi_g$ $N_2^-$ Shape Resonance using a Two Dimensional Surface and Time Dependent Wave Packet (TDWP) Approach",* International Symposium Of Molecules and Materials

(OMAM) 2009, December 28 – 29, 2009, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (Poster).

112. **B. K. Shandilya**, M. Sarma, S. Adhikari, and M. K. Mishra*, *"Time Dependent Wave Packet (TDWP) Treatment of $^2\Pi_g$ $N_2^-$ Shape Resonance using a Two Dimensional Surface for Electron – $N_2$ Interaction",* National Conference on Advances in Physical and Theoretical Chemistry, March 18 – 19, 2009, Department of Chemistry, University of Calicut, Kerala, India (Poster).

113. **M. Sarma**, S. Adhikari, and M. K. Mishra*, "*Mechanistic Analysis of Vibrational Excitation Fine Structures in e–$H_2$ Scattering*", Discussion Meeting on Theoretical Chemistry Symposium, January 18 – 22, 2009, Solid State and Structural Unit, Indian Institute of Science (IISc) Bangalore, Bangalore, India (Poster).

114. **M. Sarma**, S. Adhikari, and M. K. Mishra*, "*Some New Approaches to Photon-Molecule Dynamics*", National Symposium on Quantum Chemistry, April 04 – 05, 2008, Indian Association for the Cultivation of Science (IACS), Kolkata, India (Poster).

115. M. Sarma, R. K. Singh, and **M. K. Mishra***, "*Treatment of Vibrational Excitation Cross – sections in e – $N_2$, e – $H_2$ and e – CO Scattering Using a New Implementation of the TDWP Approach*", Singapore International Chemistry Conference 5, December 16 – 19, 2007, Singapore (Invited Talk).

116. M. Sarma, R. K. Singh, and **M. K. Mishra***, "*Local Complex Potential Based Time Dependent Wave Packet Approach to Calculation of Vibrational Excitation Cross – sections in e-$N_2$, e-$H_2$ and e-CO Scattering*", AIP Conf. Proc. **963**, 227–230 (2007) on International Conference of Computational Methods in Science and Engineering 2007 (ICCMSE 2007), Volume 2, Parts A and B, September 25 – 30, 2007, Corfu, Greece (Invited Talk).

117. M. Sarma, S. Adhikari, and **M. K. Mishra***, "*Photodynamic Control: A New Perspective*", National Symposium on Computational Chemistry, December 14 – 15, 2006, Mar Ivanios College, Thiruvananthapuram, India (Invited Talk).

118. **M. Sarma**, S. Adhikari, and M. K. Mishra*, "*Vibrationally Mediated Control of HOD Photodissociation*", National Symposium on Computational Chemistry, December 14 – 15, 2006, Mar Ivanios College, Thiruvananthapuram, India (Poster).

119. M. Sarma, S. Adhikari, and **M. K. Mishra***, "*Calculations of Vibrational Excitation Cross – section for Resonant Electron – Molecule Scattering in the Boomerang and Impulse Models*", Theoretical Chemistry Symposium (TCS) 2006, December 11 – 13, 2006, Bharthidashan University, Tiruchirappalli, India (Invited Talk).

120. **M. Sarma**, S. Adhikari, and M. K. Mishra*, "*Investigation and Control of HOD Photodissociation*", Theoretical Chemistry Symposium (TCS) 2006, December 11 – 13, 2006, Bharthidashan University, Tiruchirappalli, India (Poster).

121. **M. Sarma**, P. Ahuja, S. Adhikari, and M. K. Mishra*, "*Photodynamic Control of Chemical Reactions: Application to HOD*", In House Symposium, August 19, 2006, Chemistry Department, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Oral Talk).

122. **M. Sarma**, P. Ahuja, S. Adhikari, and M. K. Mishra*, "*Preferential Dissociation of O-D Bond in HOD Using Simple IR+UV Pulse*", Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters (SDMC), March 30 – April 01, 2006, International Center, Goa, India (Poster).

123. **M. Sarma**, P. Ahuja, S. Adhikari, and M. K. Mishra*, "*Selective Control of Photodissociation in HOD*", Current Developments in Atomic, Molecular and Chemical Physics with Applications, March 21 – 23, 2006, Physics Department, Delhi University, Delhi, India (Poster).

124. M. Sarma, P. Ahuja, S. Adhikari, and **M. K. Mishra***, "*Preferential Dissociation of O-D bond in HOD using simple IR+UV pulse*", 47$^{th}$ Sanibel Symposium, February 27 – March 03, 2006, St. Simons Island, Georgia, United States of America (Poster).

125. M. Sarma, S. Adhikari, and **M. K. Mishra***, "*Selective Control of HOD Photodissociation*", Symposium on Laser Induced Dynamics in Nano-materials and Elementary Reactions, February 13 – 14, 2006, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (Invited Talk).

126. **M. Sarma**, P. Ahuja, S. Adhikari, and M. K. Mishra*, "*New Scenarios for Vibrationally Mediated Selective Control of Bond Cleavage in HOD*", 8$^{th}$ Chemical Research Society of India – National Symposium in Chemistry, February 03 – 05, 2006, Indian Institute of Technology (IIT) Bombay, Mumbai, India (Poster).

127. **M. Sarma**, S. Adhikari, and M. K. Mishra*, "*FOIST based Control of HOD Photodissociation*", XV National Conference on Atomic and Molecular Physics, December 20 – 23, 2004, Physical Research Laboratory, Ahmedabad, India (Invited Oral Talk).

128. **M. Sarma**, S. Adhikari, and M. K. Mishra*, "*FOIST based Control of HOD Photodissociation*", Theoretical Chemistry Symposium (TCS) 2004, December 09 – 12, 2004, Bhabha Atomic Research Centre, Mumbai, India (Poster).

**General Article**

1. **M. Sarma** (2017), "Perovskite Solar Cells: Stability versus Efficiency", Curr. Sci. **113**, 840.

**Invited Talk/Popular Talk/Webinar**

1. *Exploring Cutting-Edge Research Directions in Chemistry: An Interactive Session with School Teachers of Assam*, Assam State Teachers Training Programme under Samagra Siksha Assam, December 21, 2024, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Resource Person).

2. *Career Prospects in Chemistry*, Training Program for Scientific Awareness and Career Development for School Students and Teachers, December 19, 2024, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Popular Talk).

3. *Electron-Induced Chemistry: Challenges in Computations*, Topics in Quantum Dynamics: Young Scientist Conclave, July 15 – 16, 2024, Indian Institute of Technology (IIT) Bombay, Mumbai, Maharashtra, India (Invited Talk).

4. *Theory of Unimolecular Reactions – From Collision Theory to RRKM Theory: A Journey of Four Decades*, April 25, 2024, Department of Science & Humanities, National Institute of Technology (NIT) Nagaland, Nagaland, India (Special Lecture).

5. *Photochemical Reactions of Conjugated Polyenes: Effect of Substitutions*, October 12, 2023, Department of Chemistry, Indian Institute of Technology (IIT) Bombay, Mumbai, Maharashtra, India (Invited Talk).

6. *Electron-Induced Chemistry: A Computational Perspective*, Radiation Damage to Genetic Material (RDGM) 2023, July 04 – 05, 2023, Indian Institute of Technology (IIT) Bombay, Mumbai, Maharashtra, India (Invited Talk).

7. *Advancing Careers and Exploring Cutting-Edge Research Directions in Chemistry*, Science Camp under Vigyan Jyoti Programme, June 30, 2023, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Resource Person).

8. *Theoretical Chemistry: Past, Present and Future*, June 11, 2023, 15 Minit Xikhya, Online Educational Portal, India (Online, Invited Talk).

9. *A Computational Exploration of Noncovalent Interactions in Supramolecular Host-Guest to Peptide-based Molecular Anion Receptors*, April 13, 2023, Department of Inorganic and Physical Chemistry, Indian Institute of Science (IISc) Bangalore, Bangalore, Karnataka, India (Invited Talk).

10. *Theoretical Chemistry: Quo Vadis?*, April 12, 2023, Department of Chemistry, National Institute of Technology (NIT) Surathkal, Mangalore, Karnataka, India (Invited Talk).

11. *Theoretical Chemistry: An Interplay between Structure and Dynamics*, February 03, 2023, Department of Science & Humanities, National Institute of Technology (NIT) Nagaland, Nagaland, India (Invited Talk).

12. *Career Prospects in Chemistry*, Training Program for Scientific Awareness and Career Development for School Students and Teachers, January 23, 2023, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Popular Talk).

13. *Theoretical Chemistry: Quo Vadis?*, Refresher Course in Chemistry, October 13, 2022, UGC – Human Resource Development Centre, University of Hyderabad, Hyderabad, Telangana, India (Online, Resource Person).

14. *Quantum Dynamics Application (Lecture 14)*, Ability Enhancement Program on Software Application Training Program, April 24, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

15. *Quantum Dynamics Theory (Lecture 13)*, Ability Enhancement Program on Software Application Training Program, April 24, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

16. *Applications to Density Functional Theory (Lecture 10)*, Ability Enhancement Program on Software Application Training Program, April 22, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

17. *Density Functional Theory (Lecture 09)*, Ability Enhancement Program on Software Application Training Program, April 22, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

18. *Computational Chemistry: Applications II (Lecture 08)*, Ability Enhancement Program on Software Application Training Program, April 21, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

19. *Computational Chemistry: Theory II (Lecture 07)*, Ability Enhancement Program on Software Application Training Program, April 21, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

20. *Computational Chemistry: Applications I (Lecture 06)*, Ability Enhancement Program on Software Application Training Program, April 20, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

21. *Computational Chemistry: Theory I (Lecture 05)*, Ability Enhancement Program on Software Application Training Program, April 20, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

22. *Application of Electronic Structure Theory (Lecture 04)*, Ability Enhancement Program on Software Application Training Program, April 19, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

23. *Electronic Structure Theory (Lecture 03)*, Ability Enhancement Program on Software Application Training Program, April 19, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

24. *Numerical Methods in Computational Chemistry (Lecture 02)*, Ability Enhancement Program on Software Application Training Program, April 18, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

25. *Introduction to Computational Chemistry (Lecture 01)*, Ability Enhancement Program on Software Application Training Program, April 18, 2022, Department of Chemistry, Ravenshaw University, Cuttack, India (Resource Person).

26. *Quantum Dynamics: Theory and Applications*, TEQIP – III Sponsored One-day Seminar on Theoretical and Computational Chemistry (Offline/Online), March 13, 2021, Department of Chemistry, NIT Meghalaya, Shillong, Meghalaya, India (Invited Talk).

27. *Quantum Dynamics: Theory and Applications (Lecture 02)*, Science Academies Sponsored Refresher Course on Theoretical and Computational Chemistry, February 01, 2021, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India (Online, Resource Person).

28. *Quantum Dynamics: Theory and Applications (Lecture 01)*, Science Academies Sponsored Refresher Course on Theoretical and Computational Chemistry, February 01, 2021, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India (Online, Resource Person).

29. *Electronic Structure Theory (Lecture 02)*, Science Academies Sponsored Refresher Course on Theoretical and Computational Chemistry, January 30, 2021, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India (Online, Resource Person).

30. *Electronic Structure Theory (Lecture 01)*, Science Academies Sponsored Refresher Course on Theoretical and Computational Chemistry, January 30, 2021, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India (Online, Resource Person).

31. *Numerical Methods in Theoretical Chemistry (Lecture 02)*, Science Academies Sponsored Refresher Course on Theoretical and Computational Chemistry, January 28, 2021, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India (Online, Resource Person).

32. *Numerical Methods in Theoretical Chemistry (Lecture 01)*, Science Academies Sponsored Refresher Course on Theoretical and Computational Chemistry, January 28, 2021, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, Tamilnadu, India (Online, Resource Person).

33. *Theoretical Chemistry: Quo Vadis?*, A National Webinar on Theoretical Chemistry: Quo Vadis?, August 16, 2020, Department of Chemistry and IQAC, Goalpara College, Goalpara, Assam, India (Online, Invited Talk).

34. *Theoretical Chemistry: An Interplay between Structure and Dynamics*, A National Webinar on Current Perspectives in Chemical Sciences, July 21, 2020, Department of Chemistry, Bhatter College, Dantan and Indian Chemical Society, West Bengal, India (Online, Invited Talk).

35. *Career Prospects in Chemistry*, Science Camp for Higher Secondary Students, November 08, 2019, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Popular Talk).

36. *Career Prospects in Chemistry*, Science Camp for Higher Secondary Students, August 13, 2019, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Popular Talk).

37. *Career Prospects in Chemistry*, July 26, 2019, Saraighat College, Changsari, Assam, India (Popular Talk).

38. *Interplay between Structure and Dynamics*, June 08, 2019, Department of Chemical Sciences, Tezpur University, Assam, India (Invited Talk).

39. *Low Energy Electron Induced Damage to Selected Biomolecules*, Second Edition of Jacobus Henricus van't Hoff Lecture Series, March 30 – 31, 2019, Department of Chemistry, Bodoland University, Kokrajhar, Assam, India (Invited Talk).

40. *Theoretical Chemistry: Quo Vadis?*, December 30, 2018, Department of Chemistry, Bodoland University, Kokrajhar, Assam, India (Invited Talk).

41. *Physical Chemistry: Equilibrium*, Induction Course for Newly Recruited Post Graduate Teachers of Chemistry, May 22, 2018, Navodaya Leadership Institute, Rangia, Kamrup, Assam, India. (Resource Person)

42. *Physical Chemistry: Basics of Thermodynamics*, Induction Course for Newly Recruited Post Graduate Teachers of Chemistry, May 22, 2018, Navodaya Leadership Institute, Rangia, Kamrup, Assam, India. (Resource Person)

43. *Career Prospects in Chemistry*, Workshop on Master's Entrance in Chemical Sciences – A Preparatory Guidance, February 02 – 03, 2018, IQAC and Department of Chemistry, Jorhat Kendriya Mahavidyalaya, Jorhat, Assam, India (Popular Talk).

44. *Theoretical Chemistry: Quo Vadis?*, UGC Sponsored National Seminar on Harmony with Nature in the Context of Chemistry, Environmental Issues and Challenges, September 11 – 12, 2017, Department of Chemistry, Pub Kamrup College, Baihata Chariali, Assam, India (Invited Talk).

45. *Career Prospects in Chemistry*, November 06, 2016, Indian Institute of Technology (IIT) Guwahati, Guwahati, Assam, India (Popular Talk).

**Reviewer of Journals**

- Journal of Chemical Information and Modeling
- Journal of Materials Chemistry C
- The Journal of Organic Chemistry
- Molecular Physics
- Environmental Science: Processes & Impacts
- Synthesis
- IEEE Sensors Journal
- Green Chemistry
- ACS Applied Bio Materials
- Nanoscale
- Angewandte Chemie
- Chemistry – A European Journal
- Applied Spectroscopy Reviews
- Journal of Chemical Sciences
- ACS Applied Energy Materials
- RSC Medicinal Chemistry
- ACS Applied Nano Materials
- ACS Chemical Neuroscience
- Advanced Optical Materials
- International Journal of Quantum Chemistry
- Physical Chemistry Chemical Physics
- Journal of the American Chemical Society
- Physica Scripta
- NANO
- Journal of Chemical Theory and Computation
- ChemPhotoChem
- Modern Physics Letters B
- PLOS ONE
- Chemical Science
- ACS Physical Chemistry Au
- The Journal of Physical Chemistry Letters
- Polyhedron
- Computational and Theoretical Chemistry
- Chemical Physics
- RSC Advances
- ACS Sustainable Chemistry & Engineering
- ChemPhysChem
- ACS Applied Electronic Materials
- The Journal of Physical Chemistry
- International Journal of Chemical Kinetics
- Chemical Research in Toxicology
- Bulletin of Materials Science
- Journal of Molecular Graphics and Modelling

- ACS Omega
- Journal of Indian Chemical Society
- The Journal of Physical Chemistry A

**Reviewer of PhD Thesis**

- Indian Institute of Technology (IIT) Hyderabad, Hyderabad, Telangana, India
- Osmania University, Hyderabad, Telangana, India
- University of Hyderabad, Hyderabad, Telangana, India
- Pondicherry University, Pondicherry, India
- National Institute of Science Education and Research (NISER) Bhubaneswar, Odisha, India
- National Institute of Technology (NIT) Surathkal, Mangalore, Karnataka, India
- Indian Institute of Technology (IIT) Bombay, Mumbai, Maharashtra, India
- Cotton University, Guwahati, Assam, India
- Indian Institute of Science Education and Research (IISER) Mohali, Punjab, India
- Gauhati University, Guwahati, Assam, India
- North Eastern Hill University (NEHU), Shillong, Meghalaya, India

**External Examiner/Subject Expert of PhD Thesis**

- North Eastern Hill University (NEHU), Shillong, Meghalaya, India
- Indian Institute of Technology (IIT) Hyderabad, Hyderabad, Telangana, India
- University of Hyderabad, Hyderabad, Telangana, India
- Indian Institute of Technology (IIT) Bombay, Mumbai, Maharashtra, India
- Pondicherry University, Pondicherry, India
- National Institute of Technology (NIT) Surathkal, Mangalore, Karnataka, India
- National Institute of Science Education and Research (NISER) Bhubaneswar, Odisha, India
- National Institute of Technology (NIT) Nagaland, Dimapur, Nagaland, India
- Cotton University, Guwahati, Assam, India
- Gauhati University, Guwahati, Assam, India

**External Examiner of M. Sc. Thesis**

- Gauhati University, Guwahati, Assam, India
- Tezpur University, Tezpur, Assam, India
- Indian Institute of Technology (IIT) Bhubaneswar, Odisha, India

**Curricula Review Committee**

- Member, M. Sc. (Chemistry) Curriculum Committee, National Institute of Technology (NIT) Nagaland, India

- Member, B.Tech. Curriculum Committee, International Institute of Information Technology (IIIT) Bhubaneswar, India

**Conference/Workshop/Meeting Organized**

- **One of the Organizers,** Environment 2024, December 09 – 11, 2024, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2024, December 02 – 04, 2024, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

- **One of the Conveners,** Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2024, February 22 – 25, 2024, Kaziranga, Assam, India (National).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2022, December 02 – 04, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

- **One of the Organizers,** 28$^{th}$ Chemical Research Society of India – National Symposium in Chemistry (CRSI – NSC – 28), March 25 – 27, 2022, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2018, December 06 – 08, 2018, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

- **One of the Organizers,** 5$^{th}$ International Conference on Complex Dynamical Systems and Applications (CDSA) 2017, December 04 – 06, 2017, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

- **One of the Organizers,** 20$^{th}$ Chemical Research Society of India – National Symposium in Chemistry (CRSI – NSC – 20), February 02 – 05, 2017, Gauhati University, India (National).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2016, December 08 – 10, 2016, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Mentors,** Ishan – Vikas, December 06 – 17, 2015, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** XXVII IUPAP Conference on Computational Physics (CCP) 2015, December 02 – 05, 2014, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2014, December 04 – 06, 2014, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** Fifth Programme Advisory Committee (PAC) Meeting on Physical Chemistry of Science and Engineering Research Board (SERB) New Delhi, November 11 – 13, 2013, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Conveners,** Theoretical Chemistry Symposium (TCS) 2012, December 19 – 22, 2012, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** 8$^{th}$ National Organic Symposium Trust Conference for Research Scholars (J-NOST) 2012, December 15 – 17, 2012, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2012, December 02 – 03, 2012, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** DST – SERC Winter School on Green Chemistry, March 07 – 19, 2011, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers,** Frontiers in Chemical Sciences (FICS) 2010, December 03 – 04, 2010, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (National).

- **One of the Organizers**, International Conference on Advanced Nanomaterials and Nanotechnology (ICANN) 2009, December 09 – 12, 2009, Indian Institute of Technology (IIT) Guwahati, Guwahati, India (International).

**Conference Attended/Session Chair**

- **Society of Physical Chemistry Symposium – 2025 (SoPhyC-2025)**, October 11 – 14, 2025, Session Chair, Indian Institute of Technology (IIT) Patna, Patna, India (National).

- **Structure and Dynamics: Spectroscopy and Scattering (SDSS-2023)**, October 05 – 08, 2023, Session Chair, Indian Association for the Cultivation of Science (IACS), Kolkata, India (International).

- **Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2022**, November 10 – 13, 2022, Session Chair, Malape, Karnataka, India (National).

- **Theoretical Chemistry Symposium (TCS) 2021**, December 11 – 14, 2021, Session Chair (Talk), Indian Institute of Science Education and Research (IISER) Kolkata, Mohapur, India (Online, National).

- **Online-ICNI: the Online Symposium of the International Conference on Noncovalent Interactions**, July 05, 2021, Strasbourg, France (Online, International).

- **International Conference on Spectroscopy and Dynamics of Molecular and Condensed Matter Systems (ICSD) 2020**, March 01 – 04, 2020, Puri, India (International).

- **Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2020**, February 20 – 23, 2020, Session Chair (Poster), Kumbhalgarh, Rajasthan, India (National).

- **Spectroscopy and Dynamics of Molecules and Clusters (SDMC) 2019**, February 21 – 24, 2019, Koti Resorts, Shimla, India (National).

- **Theoretical Chemistry Symposium (TCS) 2016**, December 14 – 17, 2016, University of Hyderabad, Hyderabad, India (National).

- **Current Trends in Theoretical Chemistry (CTTC) 2013**, September 26 – 28, 2013, Session Chair (Poster), Bhabha Atomic Research Centre, Mumbai, India (National).

- **Electronic Structure and Dynamics of Molecules and Clusters (ESDMC)**, February 17 – 20, 2013, Indian Association for the Cultivation of Science (IACS), Kolkata, India (International)

- **Theoretical Chemistry Symposium (TCS) 2010**, December 08 – 12, 2010, Indian Institute of Technology (IIT) Kanpur, Kanpur, India (National).

- **Recent Advances in Many Electron Theories** (RAMET) 2010, January 05 – 07, 2010, Shankarpur, West Bengal, India (National).

- **International Symposium Of Molecules and Materials** (OMAM) 2009, December 28 – 29, 2009, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, India (International).

**Workshop/Meeting/Webinar Attended**

- **ACS Science Talk**, July 24, 2020, American Chemical Society, India (National).

- **Science Writing Workshop**, August 07 – 12, 2017, Current Science Association, Bengaluru, India (National).

- **Eighty-First Meeting of the Indian Academy of Sciences Bangalore**, November 06 – 08, 2015, Indian Institute of Science Education and Research (IISER) Pune, Pune, India (National).

- **Second Platinum Jubilee Meeting of the Indian Academy of Sciences Bangalore**, November 12 – 14, 2009, Indian Institute of Science (IISc), Bangalore, India (National).

- **First Platinum Jubilee Meeting of the Indian Academy of Sciences Bangalore**, July 02 – 04, 2009, Indian Institute of Chemical Technology (IICT), Hyderabad, India (National).

**Sponsored Projects (PI / Co – PI)**

1. **Title of the Project :** Computational Designing of Next-Generation 2D TMDs/MOSs Nanohybrid Materials towards Sensing Technology (PI)

   **Total Cost :** Rs. 1,36,17,594/-

   **Agency :** Department of Science and Technology, India

   **Present Status :** Submitted

2. **Title of the Project :** Electron Attachment to Potential Radiosensitizers using a Local Complex Potential-based Time-Dependent Wavepacket Approach (PI)

   **Total Cost :** Rs. 6,60,000/-

   **Agency :** Science and Engineering Research Board (SERB), Department of Science and Technology, India

   **Present Status :** On going (2024 – )

3. **Title of the Project :** Understanding Molecular Mechanism of Calcium Signaling in Neurospora Crassa (Co – PI)

   **Total Cost :** Rs. 84,53,000/-

   **Agency :** Department of Biotechnology, India

   **Present Status :** On going (2018 – )

4. **Title of the Project :** Effect of Electron Donating and Electron Withdrawing Substituents on Single Strand Breaks in Selected DNA Fragment Induced by Low Energy Electron (PI)

   **Total Cost :** Rs. 29,46,000/-

   **Agency :** Department of Science and Technology, India

   **Present Status :** Completed (2013 – 2019)

5. **Title of the Project :** Investigation of Strand Breaks in DNA Induced by Low Energy Electron Scattering using Time Dependent Wave Packet Approach (PI)

**Total Cost :** Rs. 17,81,000/-

**Agency :** Department of Science and Technology, India

**Present Status :** Completed (2009 – 2011)

6. **Title of the Project :** Investigation of Resonances in e-$N_2$ and e-NO Scattering using 2-D Electron Nuclear Potential Energy Surfaces (PI)

   **Total Cost :** Rs. 4,25,000/-

   **Agency :** I I T Guwahati (Startup Grant)

   **Present Status :** Completed (2008 – 2010)

**Courses taught at I I T Guwahati**

- **January – May**

  **CH 232 :** Computational Chemistry (B.Tech.) [2015, 2019]
  **CH 336 :** Computational Chemistry (B.Tech.) [2009, 2010, 2011]
  **CH 501 :** Computers in Chemistry (M.Sc.) [2013, 2014, 2016, 2018]
  **CH 630 :** A Fundamental Approach to Physical Chemistry (PhD) [2017]
  **CH 634 :** Computational Methods in Chemistry (PhD) [2019]
  **CH 644 :** Applied Quantum Chemistry (B.Tech., M.Sc., PhD) [2020, 2021, 2022, 2023, 2024, 2025]

- **July – November**

  **CH 001 :** Preparatory Chemistry (Pre B.Tech.) [2015]
  **CH 101(T) :** Chemistry (Tutorial) (B.Tech.) [2009, 2010, 2012, 2013, 2014, 2015, 2016, 2017, 2018, 2019, 2023]
  **CH 110 :** Chemistry Laboratory (B.Tech.) [2012, 2015, 2016]
  **CH 231 :** Introduction to Quantum Chemistry (B.Tech.) [2012, 2018]
  **CH 402 :** Technical Writing and Seminar (B.Tech.) [2009, 2010, 2013]
  **CH 430 :** Quantum Chemistry (M.Sc.) [2017, 2019, 2020, 2023]
  **CH 435 :** Physical Chemistry Laboratory (M.Sc.) [2019]
  **CH 500 :** Graduate Seminar (M.Sc.) [2014]
  **CH 530 :** Classical and Statistical Thermodynamics (M.Sc.) [2021, 2024]
  **CH 630 :** A Fundamental Approach to Physical Chemistry (PhD) [2009, 2010]
  **CH 637 :** Computational Methods in Chemistry (PhD) [2022]
  **CH 645 :** Scientific Writing and Presentations [2025]
  **PH 305 :** Computational Physics (B. Tech.) [2013, 2014, 2016]

- **May – July**

  **CH 101 :** Chemistry (B. Tech.) [2008]

**CH 431 :** Group Theory and Spectroscopy (M.Sc.) [2008]
**CH 501 :** Computers in Chemistry (M.Sc.) [2017]

- **October 2022 – February 2023**

  **CH 101(T) :** Chemistry (Tutorial) (B.Tech.)

**Courses taught at I I T Patna**

- **August – November 2008**

  **CH 101 :** Chemistry (B.Tech.)
  **CH 101(T) :** Chemistry (Tutorial) (B.Tech.)
  **CH 110 :** Chemistry Laboratory (B.Tech.)

**Teaching Experience at I I T Bombay**

- **July – November 2005**

  **CH 101 :** Chemistry I (Tutorial) (B.Tech.)

- **July – November 2004**

  **CH 425 :** Chemical Bonding and Molecular Geometry (Integrated M.Sc.)

**Courses developed at I I T Guwahati**

- PhD Elective: **CH 645**: Scientific Writing and Presentations (3-0-0-6)
- B.Tech., M.Sc. and PhD Elective: **CH 644**: Applied Quantum Chemistry (2-0-2-6)
- PhD Elective: **CH 637**: Computational Methods in Chemistry (2-0-2-6)

**Experiments Designed at I I T Guwahati**

- **CH 435**: Physical Chemistry Laboratory – Four Experiments based on Theoretical/Computational Chemistry have been designed to provide an idea of Theoretical/Computational Chemistry to the First Year M.Sc. (Chemistry) Students

**Computer Skills**

- **Programming**: Fortran 77/90/95
- **Operating Systems**: UNIX, Windows, LINUX

**Administrative Responsibilities**

- **Chairman**, Graduate Aptitude Test in Engineering (GATE) – Joint Admission Test for Masters (JAM), 2026.

- **Coordinator**, Vigyanika – Science Literature Festival, India International Science Festival (IISF) 2024

- **Vice Chairman**, Graduate Aptitude Test in Engineering (GATE) – Joint Admission Test for Masters (JAM), 2024, 2025.

- **Paper Vetter**, Chemistry, Joint Entrance Examination (Advanced) 2022.

- **Member**, Official Language Implementation Committee, 2021 – 2024.

- **Member**, Committee for Regional Languages in Technical Education of Higher Education, 2020 –

- **Member**, Departmental Postgraduate Programme Committee (DPPC), Department of Chemistry, 2020 – 2022.

- **Member**, Departmental Space Allocation Committee, Department of Chemistry, 2020 –

- **Member**, Committee for Enhancing Community's Response to Covid-19, 2020 **–**

- **Programme Coordinator**, National Service Scheme (NSS), 2019 – 2023

- **External Member**, Departmental Postgraduate Programme Committee (DPPC), Department of Humanities and Social Sciences, 2018 – 2022.

- **Ex Officio Member**, Departmental Undergraduate Programme Committee (DUPC), Department of Chemistry, 2017 – 2020.

- **Ex Officio Member**, Departmental Postgraduate Programme Committee (DPPC), Department of Chemistry, 2017 – 2020.

- **Member**, Institute Time Table Committee (ITTC), 2017 – 2020.

- **Time Table Coordinator**, Department of Chemistry, 2017 – 2020.

- **Paper Setter**, Chemistry, Joint Admission Test for Masters (JAM), 2015.

- **Associate Warden**, Hostel Kapili, 2010 – 2011.

- **Faculty Advisor**, B.Tech. (CST) 2009 Batch, 2009 – 2011.

**Current Member of the Group**

**Post-Doctoral Fellows**

1. Dr. Juhi Dutta, National Post-Doctoral Fellow, March 2024 –

**PhD Students**

1. Ms. Ruckshana Khatun, PhD Student, Chemistry, July 2025 –
2. Mr. Madhab Morang, PhD Student, Chemistry, July 2024 –
3. Mr. Yugant P. M. Guddha, PhD Student, Centre for the Environment, July 2024 –
4. Mr. Rimi Chyrmang, PhD Student, Chemistry, July 2023 –
5. Mr. Anand Kumar Yadav, PhD Student, Chemistry, May 2023 –
6. Mr. Samsung Raja Daimari, PhD Student, Chemistry, July 2022 –
7. Mr. Manash Pratim Sarmah, PhD Student, Chemistry, July 2022 –
8. Mr. Shubham, PhD Student, Chemistry, July 2021 –
9. Mr. Rabu Ranjan Changmai, PhD Student, Chemistry, July 2019 –
10. Mr. Biman Medhi, PhD Student, Chemistry, July 2019 –
11. Ms. Monalisha Sarma, PhD Student, Chemistry, July 2019 –
12. Ms. Upasana Nath, PhD Student, Chemistry, March 2019 –
13. Ms. Niharika Keot, PhD Student, Chemistry, March 2019 –
14. Ms. Bittu Lama, PhD Student, Chemistry, July 2018 –

**PhD Students (Co-Supervisor)**

1. Ms. Udangshree Borah, PhD Student, Centre for the Environment, July 2022 –

**M. Sc. Students**

**B. Tech. Students**

1. Ms. Devashruti Saikia, B. Tech. Project Student, July 2025 –
2. Mr. Gokul Girwal, B. Tech. Project Student, July 2025 –

**Alumni of the Group**

**Post-Doctoral Fellows**

1. Dr. Juhi Dutta, Institute Post-Doctoral Fellow, December 2023 – February 2024

**PhD Students**

1. Dr. Himangshu Pratim Bhattacharyya, PhD Student, Chemistry, March 2018 – May 2025
2. Dr. Haobam Kisan Singh, PhD Student, Chemistry, July 2017 – April 2024
3. Dr. Renjith Bhaskaran, PhD Student, Chemistry, July 2009 – May 2015

**M. Sc. Students**

1. Mr. Manadip Sutradhar, M. Sc. Project Student, January 2025 – May 2025
2. Mr. Partha Sarathi Dash, M. Sc. Project Student, January 2025 – May 2025
3. Ms. Surbhi Panwar, M. Sc. Project Student, January 2023 – May 2023
4. Mr. Akhilesh Kumar, M. Sc. Project Student, January 2023 – May 2023
5. Mr. Suman Maity, M. Sc. Project Student, January 2022 – May 2022
6. Mr. Samsung Raja Daimari, M. Sc. Project Student, January 2022 – May 2022
7. Mr. Papu Kalita, M. Sc. Project Student, January 2021 – May 2021
8. Mr. Harsh Baliyan, M. Sc. Project Student, January 2021 – May 2021
9. Mr. Keshav Prasad Sahu, M. Sc. Project Student, January 2020 – May 2020
10. Mr. Deepak Kumar Saini, M. Sc. Project Student, January 2020 – May 2020
11. Mr. Sunil Kumar Patel, M.Sc. Project Student, January 2019 – May 2019
12. Mr. Nikhil Gupt, M.Sc. Project Student, January 2019 – May 2019
13. Mr. Akash Rana, M.Sc. Project Student, January 2019 – May 2019

**B. Tech. Students**

1. Mr. Mohit Adesh Patil, B. Tech. Project Student, July 2024 – May 2025
2. Mr. Trivendra Khardia, B. Tech. Project Student, July 2021 – May 2022
3. Mr. Nishu Ranjan Kumar, B. Tech. Project Student, July 2021 – May 2022
4. Mr. Kritik Rathore, B. Tech. Project Student, July 2020 – May 2021
5. Mr. Abhinav Gupta, B. Tech. Project Student, July 2020 – May 2021
6. Mr. Purushottam, B. Tech. Project Student, July 2019 – May 2020
7. Mr. Aditya Roshan, B. Tech. Project Student, July 2019 – May 2020
8. Mr. Nikhil Kumar, B. Tech. Project Student, July 2018 – May 2019
9. Ms. Nikha Garg, B. Tech. Project Student, July 2018 – May 2019
10. Mr. Ashish Kumar Agrawal, B. Tech. Project Student, July 2017 – May 2018

11. Ms. Himakshi Barsiwal, B. Tech. Project Student, July 2016 – May 2017
12. Mr. Abhijeet Anand, B.Tech. Project Student, July 2016 – May 2017

**Project Staffs**

1. Mr. Ritam Raj Borah, Project Staff, November 2019 – July 2020
2. Mr. Shyam Goswami, Project Staff, November 2015 – July 2017
3. Mr. Abdur Rahim, Project Staff, February 2014 – July 2014
4. Dr. Somnath Bhowmick, Project Staff, July 2009 – July 2012

**Summer Interns**

1. Mr. Kevizali Neikha, NIT Nagaland, June 2024
2. Ms. Anuchaya Barthakur, Tezpur University, June – July 2024
3. Ms. Kabyashree Chutia, Tezpur University, July 2023
4. Ms. Simran Kaur, Central University of Punjab, July – October 2022
5. Mr. Devesh Awasthi, IIT Kharagpur, May – July 2022
6. Mr. Rituraj Saikia, IIT Guwahati, May – July 2021 (Online)
7. Ms. Jharna Gogoi, Kaziranga University, June – July 2019
8. Mr. Chinmoy Baruah, Kaziranga University, June – July 2019
9. Mr. Rajdeep Sarma, IISER Bhopal, May – June 2019
10. Mr. Pankaj Kumar, IIT Guwahati, May – June 2019
11. Ms. Prastuti Handique, Kaziranga University, June – July 2018
12. Ms. Ankita Nandy, Kaziranga University, June – July 2018
13. Ms. Jharna Gogoi, Kaziranga University, June – July 2018
14. Ms. Dhritismita Sarma, B. Barooah College, June – July 2018
15. Ms. Nayanika Phukan, Amity University, June – July 2018
16. Mr. Praveen Kumar Sharma, Galgotias University, May – July 2018
17. Ms. Kangkana Sarma, Pub Kamrup College, May – July 2018
18. Mr. Biswajit Kalita, Pub Kamrup College, May – July 2018
19. Mr. Siddartha Kalita, Pub Kamrup College, May – July 2018
20. Ms. Barsha Chakraborty, Cotton University, July 2017
21. Ms. Moromi Nath, Pondicherry University, May – June 2017
22. Mr. Abtabh Ahmed, NISER Bhubaneswar, May – July 2017

23. Ms. Xavy Borgohain, Kaziranga University, June – July 2016
24. Ms. Sukanya Gogoi, Kaziranga University, June – July 2016
25. Mr. Saurav Mahanta, Dakshin Kamrup College, May – July 2016
26. Ms. Moghe Aditi Raman, IISER Bhopal, May – July 2016
27. Mr. Mrinal Arandhara, IIT Kharagpur, May – July 2016
28. Ms. Ansumi Gogoi, Gauhati University, July 2014
29. Ms. Susmita Burhagohain, Gauhati University, July 2014
30. Mr. Nandan Haloi, IIT Guwahati, May – July 2014
31. Mr. Rajdeep Dey, Tezpur University, May – July 2013

**Winter Interns**

1. Ms. Kabyashree Chutia, Tezpur University, December 2024 – January 2025
2. Ms. Kabyashree Chutia, Tezpur University, December 2023 – January 2024
3. Ms. Meghna Gogoi, Kaziranga University, December 2023 – April 2024 (As part of M. Sc. Project)
4. Mr. Deep Jyoti Kalita, Kaziranga University, December 2023 – January 2024 (As part of M. Sc. Project)
5. Ms. Sungjemtula Imchen, NIT Nagaland, November – December 2022
6. Mr. Kritik Rathore, IIT Guwahati, January – May 2020
7. Mr. Abhinav Gupta, IIT Guwahati, January – May 2020
8. Ms. Jharna Gogoi, Kaziranga University, January – February 2019 (As part of M.Sc. Project)
9. Ms. Suman Yadav, University of Delhi, December 2016 – January 2017
10. Ms. Madhabi Bhattacharjee, Bodoland University, December 2016 – February 2017 (As part of M.Sc. Project)
11. Ms. Karishma Talukdar, Bodoland University, December 2016 – February 2017 (As part of M.Sc. Project)

**Students Achievements**

1. Ms. Bittu Lama (PhD Student) : Selected for **PROM Program (NAWA) – Short-term Academic Exchange** to work with **Dr. Saikat Mukherjee of Nicolaus Copernicus University in Torun, Poland,** for a 28-day visit in 2025.

2. Mr. Biman Medhi (PhD Student) : Financial Assistance from Science & Engineering Research Board (SERB) under **International Travel Support (ITS) Scheme** for participating in "**CZS Summer School 2024 on Machine Learning for Chemistry, Triangel Workspace, Karlsruhe, Germany (September 09 - 13, 2024)**"
3. Ms. Bittu Lama (PhD Student) : Financial Assistance from Science & Engineering Research Board (SERB) under **International Travel Support (ITS) Scheme** for participating in "**29th IUPAC Symposium on Photochemistry (29th PhotoIUPAC), Valencia Conference Centre, Valencia, Spain (July 14 – 19, 2024)**"
4. Dr. Juhi Dutta (IPDF) : Science & Engineering Research Board (SERB) **National Post-Doctoral Fellowship**
5. Mr. Manash Pratim Sarmah (PhD Student) : One of the **Best Poster Awards** at the 17th Biennial Trombay Symposium on Radiation & Photochemistry (TSRP-2024), January 7 – 11, Bhabha Atomic Research Centre (BARC), Mumbai, India
6. Ms. Monalisha Sarma (PhD Student) : **Best Poster Award** at the Theoretical Chemistry Symposium (TCS) 2023, December 7 – 10, Indian Institute of Technology (IIT) Madras, Chennai, India
7. Mr. Himangshu Pratim Bhattacharyya (PhD Student) : Financial Assistance from Science & Engineering Research Board (SERB) under **International Travel Support (ITS) Scheme** for participating in "**6th International Conference on Molecular Simulation (ICMS 2023), National Taiwan University, Taipei, Taiwan (October 06 – 09, 2023)**"
8. Ms. Upasana Nath (PhD Student) : Financial Assistance from Science & Engineering Research Board (SERB) under **International Travel Support (ITS) Scheme** for participating in "**Graphene 2023, United Kingdom (June 27 – 30, 2023)**"
9. Mr. Manash Pratim Sarmah (PhD Student) : **Prime Minister's Research Fellows (PMRF)**, 2022
10. Mr. Shubham (PhD Student) : **Prime Minister's Research Fellows (PMRF)**, 2022
11. Mr. Rabu Ranjan Changmai (PhD Student) : **Best Poster Award** at the Current Trends in Theoretical Chemistry (CTTC-2022), September 22 – 24, Bhabha Atomic Research Centre (BARC), Mumbai, India

12. Mr. Papu Kalita (M. Sc. Project Student) : **Institute Silver Medal** for securing First Position in M. Sc. Chemistry in 2021 (awarded by IIT Guwahati)
13. Mr. Abhinav Gupta (B.Tech. Project Student): **Samsung Fellowship** to carry out the translational research from April – June 2021

**Research Collaborators (Abroad)**

1. Professor Pavel Hobza, Institute of Organic Chemistry and Biochemistry ASCR, Prague (Czech Republic)
2. Dr. Amrit Sarmah, Associate Scientist, Department of Molecular Modelling, Institute of Organic Chemistry and Biochemistry ASCR, Prague (Czech Republic)
3. Professor Ricardo A. Mata, Institut für Physikalische Chemie, Universität Göttingen (Germany)

**Research Collaborators (India)**

1. Professor Anil Kumar Saikia, Department of Chemistry, IIT Guwahati (India)
2. Professor Mohammad Qureshi, Department of Chemistry, IIT Guwahati (India)
3. Professor Bhubaneswar Mandal, Department of Chemistry, IIT Guwahati (India)
4. Dr. Monali Dutta Saikia, Arya Vidyapeeth College, Guwahati (India)
5. Professor Md. Akhtarul Alam, Department of Chemistry, Aliah University (India)
6. Dr. Biswajit Saha, Materials Science & Technology Division, CSIR-North East Institute of Science & Technology, Jorhat (India)
7. Dr. Pradip Maity, Organic Chemistry Division, CSIR-National Chemical Laboratory, Pune (India)
8. Professor Pravat Kumar Giri, Department of Physics, IIT Guwahati (India)
9. Professor Kaushik Ghosh, Department of Chemistry, IIT Roorkee (India)
10. Dr. Pankaj Kalita, School of Energy Science and Engineering, IIT Guwahati (India)
11. Dr. Basanta Kumar Rajbongshi, Department of Chemistry, Cotton University (India)
12. Dr. Pranjal Kumar Baruah, Department of Applied Sciences, Gauhati University (India)
13. Dr. Prasanta Jyoti Goutam, Department of Chemistry, Kaziranga University (India)

**References**

1. **Professor Manoj K. Mishra**
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   Ex-Vice Chancellor, BIT Mesra, Ranchi
   Ex-Vice Chancellor, Lucknow University
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