Dr. Lisa Roy

Assistant Professor Grade I (Chemistry)
Department of Education
Indian Institute of Technology, Kharagpur
Kharagpur, 721302. India
Email: L.Roy@edu.iitkgp.ac.in

Google Scholar | ORCiD | Personal Homepage
ResearchGate | LinkedIn | Twitter

Educational Qualification

- **Ph.D(Science) in Chemistry (2015)** from Indian Association for the Cultivation of Science, Kolkata. (Degree received from University of Calcutta). Thesis Title: *Theoretical Investigation of Reaction Mechanisms of Chemical Reactions Related to Renewable Energy*. Supervisor: Prof. Ankan Paul. Specialization: ***Computational Chemistry***

- **M. Sc. in Chemistry (2009)** from University of Calcutta, Kolkata. Specialization: ***Physical Chemistry***. First Class with Grade "A+." *Stood first in the Physical Chemistry section*. Master's Project Title: *Locating Global Minimum in a Rugged Landscape using a Modified Deterministic Strategy*. Supervisor: Prof. Pinaki Chaudhury

- **B.Sc (Hons.) in Chemistry (2007)** from Vivekananda College affiliated to University of Calcutta, Kolkata. Minor subjects: Physics, Mathematics. First Class. *Stood second in the Department of Chemistry*.

Professional Experience

- **Assistant Professor Grade I** (since August 2024)
  Indian Institute of Technology, Kharagpur

- **Assistant Professor** (November 2018 - August 2024)
  Institute of Chemical Technology Mumbai - IOC Odisha Campus Bhubaneswar

- **DST INSPIRE Faculty Fellow** (October 2017- October 2018)
  CSIR Central Mechanical Engineering Research Institute, Durgapur

- **Postdoctoral Researcher** (July 2015 – October 2017)
  Max Planck Institute for Chemical Energy Conversion, Germany
  Research Group of Prof. Frank Neese; Group leader Prof. Shengfa Ye

Awards and Honors

- Jury Member, Chemistry Europe Award (Chemistry Europe Society, Wiley VcH), 2024
- CSIR ASPIRE Extramural Research Grant, 2024
- Certificate of Excellent Grade in Performance Review Meeting by DST INSPIRE (2023)
- Early Career Advisory Board Member of *ChemPhysChem* (Chemistry Europe Society, Wiley VcH) Jan 2023-present
- SERB POWER (Promoting Opportunities for Women in Exploratory Research) Grant, 2021
- Early Career Advisory Board Member of *ChemPlusChem* (Chemistry Europe Society, Wiley VcH) Jan 2021-present
- Visiting Researcher at the Max Planck Institute for Coal Research, Germany (July 2019)
- DST INSPIRE Faculty Fellowship (2017) in Chemical Sciences Division
- Offered Postdoctoral Fellowship at The Hebrew University of Jerusalem (2017) (not availed)
- Max-Planck Postdoctoral Fellowship July 2015 – Oct 2017
- International Travel Support from SERB in 2012 for participating at the 48th STC held at KIT in Germany
- Qualified the Graduate Aptitude Test in Engineering in 2010
- Qualified the Joint CSIR-UGC National Eligibility Test 2009, CSIR fellowship JRF/SRF from July 2010 – June 2015
- Qualified State Eligibility Test (2009) held by West Bengal College Service Commission for Lectureship
- Awarded Motilal Nath Award (2007) by Vivekananda College for excellence in B.Sc examination

Research Interests

Our primary research interest lies in the broad area of catalysis which include reactivity study of metalloenzyme and model complexes, organo-catalysts, and metal-organic-frameworks/covalent-organic-frameworks to computationally design novel catalytic systems for sustainable energy and resources. We mainly use combined density functional and wave-function based methods like the multireference and local pair natural orbital coupled cluster techniques and semi-empirical tight binding approaches to deliver a reliable picture of the catalyst active site binding, aggregation, and reaction mechanism. We are mainly focused on three different sub-topics:

- Bio-inspired C-H activation or C=C hydroxylation
- Small molecule activation by 3d transition metal
- Non-covalent interaction assisted catalysis

List of Publications

Peer-Reviewed Journals:

1. *Changing Lanes from Concerted to Stepwise Hydrogenation: The Reduction Mechanism of Frustrated Lewis Acid–Base Pair Trapped CO_2 to Methanol by Ammonia–Borane*
Lisa Roy, Paul M. Zimmerman and Ankan Paul*. ***Chem. Eur. J.*** 2011, 17, 435-439.

2. *Breaking the Myth of the Recalcitrant Chemisorbed Hydrogens on Boron Nitride Nanotubes: A Theoretical Perspective*
Lisa Roy, Samyak Mittal and Ankan Paul*. ***Angew. Chem. Int. Ed.*** 2012, 51, 4152-4156.

3. *The Role of Solvent and of Species Generated in Situ on the Kinetic Acceleration of Aminoborane Oligomerization*
Tanmay Malakar, **Lisa Roy** and Ankan Paul*. ***Chem. Eur. J.*** 2013, 19, 5812-5817.

4. *Self-Assembly of Carboxylic Acid-Appended Naphthalene Diimide Derivatives with Tunable Luminescent Color and Electrical Conductivity*
Mijanur Rahaman Molla, Dominik Gehrig, **Lisa Roy**, Valentin Kamm, Ankan Paul*, Frederique Laquai and Suhrit Ghosh*. ***Chem. Eur. J.*** 2014, 20, 760-771.

5. *A metal free strategy to release chemisorbed H_2 from hydrogenated Boron Nitride nanotubes*
Lisa Roy, Sourav Bhunya and Ankan Paul*. ***Angew. Chem. Int. Ed.*** 2014, 53, 12430-12435.

6. *Computational design of an Iridium based catalyst for releasing H_2 from hydrogenated BN nanotubes*
Lisa Roy* and Ankan Paul*. ***Chem. Commun.*** 2015, 51, 10532-10535.

7. *A Serendipitous Rendezvous with a Four-Center Two-Electron Bonded Intermediate in the Aerial Oxidation of Hydrazine*
Ambar Banerjee, Gaurab Ganguly, **Lisa Roy**, Shubhrodeep Pathak and Ankan Paul*. ***Chem. Eur. J.*** 2016, 22, 1216-1222. (Selected for *Frontispiece*)

8. *Mechanistic Details of Ru-bispyridylborate complex catalyzed dehydrogenation of ammonia-borane: The Role of pendant Boron Ligand in catalysis*
Sourav Bhunya, **Lisa Roy** and Ankan Paul*. ***ACS Catal.*** 2016, 6, 4068-4080.

9. *High-Valent Iron-Oxo and-Nitrido Complexes: Bonding and Reactivity*
Bhaskar Mondal, **Lisa Roy**, Frank Neese and Shengfa Ye*. ***Isr. J. Chem.*** 2016, 56, 763-772. (***Invited*** *for a Special Issue entitled New Frontiers in Bioinorganic Chemistry***)**

10. *Ligand Rearrangements at Fe/S Cofactors: Slow Isomerization of a Biomimetic [2Fe-2S] Cluster*
Marie Bergner, **Lisa Roy**, Sebastian Dechert, Frank Neese, Shengfa Ye* and Franc Meyer*. ***Angew. Chem. Int. Ed.*** 2017, 56, 4882-4886. ***(HOT Paper)***

11. *Lewis Acid Promoted Hydrogenation of CO_2 and $HCOO^-$ by Amine Boranes: Mechanistic Insight from a Computational Approach*
Lisa Roy*, Boyli Ghosh and Ankan Paul*. ***J. Phys. Chem. A*** 2017, 121, 5204-5216.

12. *Theoretical Insights into the Nature of Oxidant and Mechanism in the Regioselective Syn-dihydroxylation of an Alkene*

with a Rieske oxygenase inspired Iron Catalyst
Lisa Roy*. ***ChemCatChem*** 2018, 7, 3683-3688.

13. *Reduction of CO_2 by a Masked Two-Coordinate Cobalt(I) Complex and Characterization of a Proposed Oxodicobalt(II) Species*
Lisa Roy, Malik H. Al-Afyouni, Daniel E. DeRosha, Bhaskar Mondal, Ida M. DiMucci, Kyle M. Lancaster, Jason Shearer, Eckhard Bill, William W. Brennessel, Frank Neese, Shengfa Ye* and Patrick L. Holland*. ***Chem. Sci.*** 2019,10, 918-929.

14. *Theoretical Identification of the Factors Governing the Reactivity of C-H Bond Activation by Non-Heme Iron(IV)-Oxo Complexes*
Lisa Roy*. ***ChemPlusChem*** 2019, 84, 893-906. (Selected for ***ChemPlusChem Readers' Choice 2019 and 2020*****)**

15. *Structurally Tunable pH-Responsive Luminescent Assemblies from Halogen Bonded Supra-π-Amphiphiles*
Akshoy Jamadar, Chandan Kumar Karan, **Lisa Roy** and Anindita Das*. ***Langmuir*** 2020, 36, 3089-3095.

16. *Unravelling the possibility of hydrogen storage on Naphthalene Dicarboxylate based MOF linkers: A Theoretical Perspective*
Pratibha Agarwala, Saswat Kumar Pati and **Lisa Roy***, ***Mol. Phys.*** 2020, 118, e1757169. (Invited for a *Special Issue* entitled *MQM2019*)

17. *Theoretical Investigation of an Acid Catalyst for Viable Release of H_2 from BN Nanotubes: A Local Pair Natural Orbital Coupled Cluster Approach*
Lisa Roy*. ***Int. J. Quantum Chem.*** 2020, 120, e26257.

18. *Alcohols as Fluoroalkyl Synthons: Ni-catalyzed Dehydrogenative Approach to Access Polyfluoroalkyl Bis-indoles*
V. Arun, **Lisa Roy*** and Suman De Sarkar*, ***Chem. Eur. J.*** 2020, *26*, 16649 – 16654.

19. *Computational Mechanistic Insights into Non-noble Metal Catalysed CO_2 Conversion*
Lisa Roy, Bhaskar Mondal and Shengfa Ye, ***Dalton Trans.*** 2020, 49, 16608 – 16616.

20. *Computational Investigation of the Mechanism of FLP Catalyzed H_2 Activation and Lewis Base Assisted Proton Transfer*
Munia Sultana, Ankan Paul and **Lisa Roy***, ***ChemistrySelect*** 2020, 5, 13397 – 13406. (Selected for a *Special Issue* entitled *Catalysis*)

21. *Organophotoredox-catalyzed redox-neutral cascade involving N-(acyloxy)phthalimides and maleimides*
Sanju Das, Sushanta Kumar Parida, Tanumoy Mandal, Sudhir Kumar Hota, **Lisa Roy***, Suman De Sarkar* and Sandip Murarka*, ***Org. Chem. Front.*** 2021, 8, 2256 – 2262.

22. *The C_{sp}-C_{sp} Bond Cleavage and Fragments Coupling: Transition Metal-Free "Extrusion and Recombination" Approach towards Synthesis of 1,2-Diketones*
Raghuram Gujjarappa, Nagaraju Vodnala, Ashish Kandpal, **Lisa Roy**, Sreya Gupta and Chandi C. Malakar*, ***Org. Chem. Front.*** 2021, 8, 5389-5396.

23. *Stimuli-Responsive Luminescent Supramolecular Assemblies and Co-assemblies by Orthogonal Dipole-Dipole Interaction and Halogen Bonding*
Akshoy Jamadar, Ajeet Kumar Singh, **Lisa Roy*** and Anindita Das*, ***J. Mater. Chem C*** 2021, 9, 11893-11904. (Selected for part of themed collection: *Journal of Materials Chemistry C Emerging Investigators*)

24. *Unconventional Ethereal Solvents in Organic Chemistry: A Perspective on Applications of 2-Methyltetrahydrofuran, Cyclopentyl Methyl Ether, and 4-Methyltetrahydropyran*
Rachel Bijoy, Pratibha Agarwala, **Lisa Roy**, Bhaskar N. Thorat*, ***Org. Process Res. Dev.*** 2022, 26, 480-492. (Selected for Most Read Chemistry Articles of November 2021 by *ACS Axial*)

25. *Trifluoroethanol as a Unique Additive for the Chemoselective Electrooxidation of Enamines to Access Unsymmetrically Substituted NH-Pyrroles*
Mrinmay Baidya, Debabrata Maiti, **Lisa Roy***, Suman De Sarkar*, ***Angew. Chem. Int. Ed.*** 2022, 61, e202111679. ***(Hot Paper)***

26. *Luminescent property switching in 1D supramolecular polymerization of organic donor- π-acceptor chromophore*
Sk Mursed Ali, Subrata Santra, Arun Mondal, Soumya Koley, **Lisa Roy**, Mijanur Rahaman Molla*, ***Polym. Chem.*** 2022, 13, 558 – 568.

27. *Nonequilibrium Catalytic Supramolecular Assemblies of Melamine- and Imidazole-Based Dynamic Building Blocks*
Syed Pavel Afrose, Chiranjit Mahato, Pooja Sharma, **Lisa Roy**, Dibyendu Das*, ***J. Am. Chem. Soc.*** 2022, 144, 673 – 678.

28. *The Role of Copper Salts and O_2 in the Mechanism of C≡N Bond Activation for Facilitating Nitrogen Transfer Reactions*
Boyli Ghosh, Ambar Banerjee, **Lisa Roy**, Rounak Nath, Rabindra Nath Manna, Ankan Paul*, ***Angew. Chem. Int. Ed.*** 2022, 61, e202116868.

29. *An Expeditious Route to Sterically Encumbered Nonproteinogenic α-Amino Acid Precursors Using Allylboronic Acids*
Samrat Sahu, Ganesh Karan, **Lisa Roy**, Modhu Sudan Maji*, ***Chem. Sci.*** 2022, 13, 2355 – 2362.

30. *Solvophobically-Driven Merocyanine Dye Assembly: Predominant Dipole-Dipole Interactions Over Hydrogen-Bonding*
Aritra Rajak, Ajeet Kumar Singh, **Lisa Roy***, Anindita Das*, ***ChemNanoMat*** 2022, 8, e202200082.

31. *Supramolecularly cross-linked nanoassemblies of self-immolative polyurethane from recycled plastic waste: high encapsulation stability and the triggered release of guest molecules*
Subrata Santra, Soumya Kolay, Sujauddin Sk, Debleena Ghosh, Anmol Mishra, **Lisa Roy**, Kishor Sarkar and Mijanur Rahaman Molla*, ***Polym. Chem.*** 2022,13, 3294-3303.

32. *Stabilizing Entropically Driven Self-Assembly of Self-Immolative Polyurethanes in Water: A Strategy for Tunable Encapsulation Stability and Controlled Cargo Release*
Subrata Santra, Arpan Ghosh, Arun Mondal, Sk Mursed Ali, Dishan Das, Kishor Sarkar, **Lisa Roy**, and Mijanur Rahaman Molla*, ***ACS Appl. Polym. Mater.*** 2022, 4, 7614–7625.

33. *Development of Carbazole-Cored Organo-Photocatalyst for Visible Light-Driven Reductive Pinacol/Imino-Pinacol Coupling*
Samrat Kundu, **Lisa Roy**, Modhu Sudan Maji*, ***Org. Lett.*** 2022, 24, 9001–9006.

34. *Tuning of the Supramolecular Helicity of Peptide-Based Gel Nanofibers*
Souvik Mishra, Pijush Singh, Ajeet Kumar Singh, **Lisa Roy**, Soumen Kuila, Sukantha Dey, Ajit K. Mahapatra, Jayanta Nanda*, ***J. Phys. Chem. B*** 2022, 126, 10882–10892

35. *Zn(II)-Catalyzed Selective N-Alkylation of Amines with Alcohols using Redox Noninnocent Azo-aromatic Ligand as Electron and Hydrogen Reservoir*
Subhajit Chakraborty, Rakesh Mondal, Subhasree Pal, Amit Kumar Guin, **Lisa Roy*,** and Nanda D. Paul*, ***J. Org. Chem.*** 2023, 88, 771–787.

36. *Photoinduced Electron Donor-Acceptor Complex-mediated Radical Cascade Involving N-(acyloxy)phthalimides: Synthesis of Tetrahydroquinolines*
Sudhir Kumar Hota, Satya Prakash Panda, Sanju Das, Sanat Kumar Mahapatra, **Lisa Roy***, Suman De Sarkar*, and Sandip Murarka*, ***J. Org. Chem.*** 2023, 88, 2543-2549.

37. *Pathway Complexity in Supramolecular Copolymerization and Blocky Star Copolymers by a Hetero-Seeding Effect*
Payel Khanra, Ajeet Kumar Singh, **Lisa Roy**, and Anindita Das*, ***J. Am. Chem. Soc.*** 2023, 145, 5270-5284.

38. *A convenient route to vinylogous dicyano aryl based AIEgen with switchable mechanochromic luminescence property*
Saurajit Ghosh, Himanshi Bhambri, Ajeet Kumar Singh, Sanjay Mandal, **Lisa Roy**, Partha S Addy*, ***Chem. Commun.*** 2023, 59, 4463–4466.

39. *Pd(II)-Catalyzed Oxidative Naphthylation of 2-Pyridone through N–H/C–H Activation Using Diarylacetylene as an Uncommon Arylating Agent*
Satabdi Bera, Aniruddha Biswas, Juthi Pal, **Lisa Roy**, Supriya Mondal, and Rajarshi Samanta*, ***Org. Lett.*** 2023, 25, 1952−1957.

40. *Photodecarboxylative C–H Alkylation of Azauracils with N-(Acyloxy)phthalimides*
Satya Prakash Panda, Sudhir Kumar Hota, Rupashri Dash, **Lisa Roy** and Sandip Kumar Murarka*, ***Org. Lett.*** 2023, 25, 3739 – 3744.

41. *Probing Molecular Chirality on the Self-Assembly and Gelation of Naphthalimide-Conjugated Dipeptides*
Soumen Kuila, Ajeet Kumar Singh, Akash Shrivastava, Sukantha Dey, Tukai Singha, **Lisa Roy**, Biswarup Satpati and Jayanta Nanda*, ***J. Phys. Chem. B*** 2023, 127, 21, 4808–4819.

42. *Computational Mechanistic Insights on Homogeneous Water Oxidation Versus Catalyst Deactivation: A Case Study with Mononuclear Nickel and Copper Complexes*
Ajeet Kumar Singh and **Lisa Roy***, ***Eur. J. Inorg. Chem.*** 2023, 26, e202300412 (***Invited*** *for a Special Collection on Inorganic Reaction Mechanisms*) *(**Cover Feature**)* (*Special Collection on Evolving with Inorganic Chemistry for 25 Years*)

43. *Structurally Divergent Enantioselective Synthesis of Benzofuran Fused Azocine Derivatives and Spiro-Cyclopentanone Benzofurans Enabled by Sequential Catalysis*
Rupkumar Khuntia, Sanat Kumar Mahapatra, **Lisa Roy** and Subhas Chandra Pan*, ***Chem. Sci.*** 2023,14, 10768-10776.

44. A General Electron Donor–Acceptor Photoactivation Platform of Diaryliodonium Reagents: Arylation of Heterocycles
Prahallad Meher, Satya Prakash Panda, Sanat Kumar Mahapatra, Karan Ramdas Thombare, **Lisa Roy*** and Sandip Murarka*, ***Org. Lett.*** 2023, 25, 8290–8295.

45. Cu(II) promoted C(sp^3)-H activation in unactivated cycloalkanes: Oxo-alkylation of styrenes to synthesize b-disubstituted ketones
Krishna Mohan Das, Adwitiya Pal, Lakshmi Surya T, **Lisa Roy,** and Arunabha Thakur*, ***Chem. Eur. J.***, 2024, 30, e202303776.

46. Divergent Electrochemical Synthesis of Indoles through pKa Regulation of Amides: Synthetic and Mechanistic Insights
Samrat Mallick, Tanumoy Mandal, Nidhi Kumari, **Lisa Roy*,** and Suman De Sarkar, ***Chem. Eur. J.***, 2024, e202304002 ***(Hot Paper)***

47. Evolution in the Design of Water Oxidation Catalysts with Transition-Metals: A Perspective on Biological, Molecular, Supramolecular and Hybrid Approaches
Ajeet Kumar Singh and **Lisa Roy*,** ***ACS Omega*** 2024, 9, 9886–9920. ***(Invited, Selected for Supplementary Cover)***

48. Experimental and theoretical insights for designing Zn2+ complexes to trigger chemo-selective hetero-coupling of alcohols
Arup Samanta, Prativa Behera, Amit Chaubey, Avijit Mondal, Debjyoti Pal, Kailash Mohar, **Lisa Roy***, and Dipankar Srimani*, ***Chem. Commun.,*** 2024, 60, 4056-4059

49. Silylarylation of Alkenes via meta-Selective C-H Activation of Arenes under Ruthenium/Iron Cooperative Catalysis: Mechanistic Insights from Combined Experimental and Computational Studies
Sukanya Neogi,‡ Sourav Bhunya,‡ Asim Kumar Ghosh, Biswajit Sarkar, **Lisa Roy**, and Alakananda Hajra (‡ These authors contributed equally), ***ACS Catal.*** 2024, 14, 4510-4522

50. Rh(II)-Catalysed N2-Selective Arylation of Benzotriazoles and Indazoles using Quinoid Carbenes via 1,5-H Shift
Souradip Sarkar, Sourav Bhunya,‡ Subarna Pan,‡ Arnadeep Datta, **Lisa Roy*,** and Rajarshi Samanta* (‡ These authors contributed equally), ***Chem. Commun.,*** 2024, 60, 4727-4730.

51. Toward Rational Design of Mononuclear Nickel Complexes as Water Oxidation Catalysts Exploring the Ligand Effects on the Rate-Determining Step
Ajeet Kumar Singh, **Lisa Roy*,** ***ChemPhysChem***, 2024. DOI: 10.1002/cphc.202400533 (Accepted)

52. Alkoxide Assisted Stereoselective Functionalization of 1,2-Bis-boronic Esters Under Photoredox Catalysis
Somenath Mahato, Debraj Ghorai, Kanak Kanti Das, **Lisa Roy**, and Santanu Panda*, ***Org. Lett.*** 2024 (Accepted), DOI: 10.1021/acs.orglett.4c02469

53. Manganese catalyzed chemo-selective synthesis of acyl cyclopentenes: a combined experimental and computational investigation

Koushik Sarkar, Prativa Behera, **Lisa Roy*** and Biplab Maji*, ***Chem. Sci.,*** 2024 (Accepted), DOI: 10.1039/D4SC02842B

Book Chapter:

1. *Theoretical Approach to Homogeneous Catalytic Reduction of CO_2: Mechanistic Understanding to Build New Catalysts* **Lisa Roy**, Bhaskar Mondal, Frank Neese and Shengfa Ye, *Chapter 5*, pages 197 – 225, Carbon Dioxide Electrochemistry: Homogeneous and Heterogeneous Catalysis, ***Royal Society of Chemistry***, 2020.

2. Transition Metals and Their Complexes as Homogeneous Catalysts
Prativa Behera and **Lisa Roy***, *Chapter 8*, Adv. in Cat. Vol. 1 - Homogeneous Catalysis Concepts and Basics, ***Elsevier***, 2024.

Teaching Experience

- **M.Sc Chemistry at ICT-IOCB**
  2024: *Supramolecular Chemistry (Elective): Nature of binding interactions in supramolecular structures, Host-Guest interactions, crown ethers, cryptands, calixarenes, cyclodextrins and other supramolecular structure, role of H-bonding and other weak interactions in crystal engineering, Self-assembly of molecules, Relevance of supramolecular chemistry to mimic biological systems, Examples of recent developments from current literature.*
  2023: *Chemical Dynamics*: *Kinetics and reaction mechanism, Theories of reaction rates – Collision theory, Transition State theory, solvent effects and diffusion-controlled reactions, Activation, and diffusion-controlled processes- Marcus Kinetics, Experimental techniques for measuring kinetics of fast reactions etc.*
- **Basic Science Course for Integrated MTech at ICT-IOCB**
  2023: *Chemical Kinetics and Catalysis*
  2022: (1) *Computational Chemistry Elective* (T): *Quantum Mechanics such as Hartree-Fock and post-Hartree-Fock methods, molecular dynamics simulations, force-field based approaches*. (2) Food Chemistry Minor (T): *Biochemistry of components such as Liquid Water and Ice, their activity and phase transitions; configuration, conformation and physical properties of carbohydrates, sequences, conformation, and helical structures of proteins* etc. (3) Chemical Kinetics and Catalysis
  2021: Chemistry I (T): *Bonding in transition metal complexes, organometallic reaction mechanisms, nuclear chemistry, spectroscopic and chromatographic analysis;* Chemistry I (P): *Analytical and physical chemistry experiments*
  2020: Chemistry II (T): *Chemical Kinetics, Surface and interfacial chemistry, Catalysis, Electrochemistry*; Chemistry II (P): *Acid-base titrations, chemical kinetics experiments*
  2019: Chemistry II (T): *Physical organic chemistry, aromaticity, reaction mechanisms*; Chemistry II (P) *Synthesis of organic compounds by green chemistry approach*
  2018: Chemistry I (T): *Spectroscopy and analytical chemistry*; Chemistry I (P): *Analytical experiments with spectrophotometer, colorimeter, pH meter etc.*
- **PhD Coursework** undertaken at CSIR-CMERI for August 2018 session: Advanced Material Science
- **Tutor** in Summer Schools, Gelsenkirchen, Germany (2015, 2016, 2017) oriented towards computational reactivity and spectroscopy study with the ORCA program package.

Research Guidance

- Currently supervising Ajeet Kumar Singh (PhD Research Scholar), Sanat Kumar Mahapatra (PhD Research Scholar), Prativa Behera (PhD Research Scholar), Saitosh Mohanty (M.Sc project student)
- Past students: Lakshmi Surya T (Project Junior Research Fellow), Praseetha Prakash (Project Junior Research Fellow), Dishan Das (Research Intern), Pousali Mitra (Project Assistant), Anmol Mishra (Research Intern), Hritwik Haldar (Autumn Intern), Lalita Mehra (Summer Intern), Ashish Kandpal (Project Assistant), Pratibha Agarwala (Project Assistant), Anindita Chandra (Project Assistant) and Saswat Kumar Pati (B.S Intern)

Poster Presentations

1. Mechanistic Investigations of reduction of frustrated Lewis pair trapped CO_2 by ammonia-borane and related reactions at the Theoretical Chemistry Symposium (TCS2010), IIT Kanpur, India, December 2010.

2. *Concerted dehydrocoupling of chemisorbed hydrogens on Boron Nitride nanotubes and fullerenes: A density functional investigation* at the 48th Symposium on Theoretical Chemistry, Karlsruhe Institute of Technology, Germany, September 2012.

3. *Dehydrocoupling of chemisorbed hydrogens from BN nanotubes: Implications in hydrogen storage* at DAE-BRNS

symposium on Current Trends in Theoretical Chemistry (CTTC-2013), Bhabha Atomic Research Centre, India, September 2013.

4. *C-H activation by Model Di-iron Complexes: A DFT study* at Gordon Research Conference for Computational Chemistry, Girona, Spain, July 2016

5. *C-H Bond Activation by Model Diiron Complexes: A DFT Study* at the 52nd Symposium on Theoretical Chemistry, Ruhr University Bochum, Germany, September 2016

6. *Metal-Metal Cooperativity in the Co(I) Mediated Reductive Disproportionation of CO2 to Carbonate (CO32-) and Carbonyl (CO)* at the 15th Indian Theoretical Chemistry Symposium (TCS2016), University of Hyderabad, India, December 2016

7. *Effects of core geometries and local spin states on the reactivity of high-valent iron complexes* at Gordon Research Conference for Metals in Biology, Ventura, USA, January 2017.

8. *Variable C-H Activation by High-Valent Fe_2-μ-Oxo Complexes Featuring Open- or Diamond Cores: An Interplay between Core Geometry Effects and Spin States* at Fem-Ex NL 2017, Putten, Netherlands, June 2017.

9. *Quantum Chemical Exploration of Transition Metal Mediated CO_2 Disproportionation and Hydrogenation* at the 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany, August 2017.

10. *Elucidation of the Reaction Mechanism of Copper Catalyzed Water Oxidation* at Asia Pacific Conference in Theoretical and Computational Chemistry, IIT Bombay, India, December 2017.

11. *Non-noble metal catalyzed CO_2 conversion: from mechanistic understanding to new catalyst design* at India International Science Festival, Young Scientists' Conference, Kolkata, November 2019

12. Invited Poster on *Computational Insights into Manganese Catalyzed Vinyl Cyclopropane Ring Expansion Cascade* International Conference on Organometallics and Catalysis, organized by IISC Bangalore, IIT Bombay and IISER Kolkata at Goa, India October 2023

Seminars/Lectures

1. Invited talk on *Theoretical Perspective of BN Nanotube/Fullerene based Hydrogen Storage beyond Ammonia Borane* at National Conference on Graphene and Functional Materials, CSIR CMERI, Durgapur, February 2018.

2. Invited talk on *Unraveling the Mechanistic Intricacies of Transition Metal Mediated H_2 formation, CO_2 reduction and C-H activation* at BITS Pilani, Hyderabad Campus, India, April 2018

3. Invited talk on *Theoretical Insights into The Nature of Oxidant and Mechanism in Bioinspired Non-Heme Iron Catalyzed C-H/C=C Bond Oxidation* at the 16th Theoretical Chemistry Symposium, BITS Pilani, February 2019

4. Contributed talk on *Theoretical Insights into The Nature of Oxidant and Mechanism in Bioinspired Non-Heme Iron Catalyzed Reactions* at 9th Molecular Quantum Mechanics, Heidelberg, Germany, July 2019.

5. Invited talk on *Theoretical Insights into The Nature of Oxidant and Mechanism in Bioinspired Non-Heme Iron Catalyzed Reactions* at Max Planck Institute for Coal Research, Germany, July 2019

6. Invited lecture on *Catalysis in Computers: Mechanistic Insights on CO_2 Reduction, C-H Activation and C=C Oxidation* at Five Days National Webinar under TEQIP-III on "The Chemistry in Fume Hood to Computers" organized by NIT Manipur, November 2020

7. Invited talk on *Computational Mechanistic Insights into Bio-Inspired Homogeneous Catalytic Reduction of CO_2* at ChemSci2020 – Leaders in the Field Symposium jointly organized by Royal Society of Chemistry and IISER Kolkata, December 2020

8. Contributed talk on *Theoretical Insights on Non-Covalent Interaction Assisted Catalysis and Supramolecular Assembly* at India International Science Festival – Young Scientists' Conference, December 2020

9. Key Note Lecture on *Catalysis in Computers: Mechanistic Insights for CO_2 Utilization* at Advances in Carbon Dioxide Capture & Utilization for Sustainable Climate (ACCUSC – 2022) organized by NIT Rourkela, July 2022.

10. Invited talk on *Computational Investigations of Non-covalent Interactions Assisted Catalysis* at Designing Catalysts on Computers (DCC - 2022) organized by IACS, Kolkata, December 2022.

11. Invited flash talk on *Harnessing Non-Covalent Interactions* at Indo-French Seminar on Catalysis for Sustainability, jointly organized by IISER-TVM, IIT-Kanpur & LCC-Toulouse, IISER TVM, December 2023.

12. Invited lecture on *Harnessing Non-covalent Interaction in Catalysis: From Molecules to Supramolecules* at DAE-BRNS National Workshop on Atomistic Modeling of Molecules and Materials (AMMM-2023), BARC Mumbai, December 2023.

13. Invited talk on *A Computational Perspective on Harnessing Non-covalent Interactions in Catalysis* at IIT Bombay, January 2024

14. Invited talk on *Harnessing Non-covalent Interaction in Catalysis at Organic Chemistry* Symposium at Synthesis, Catalysis and Chemical Biology organized by ICT Mumbai, January 2024.

15. Invited talk on *A Computational Mechanistic Perspective on Harnessing Non-covalent Interactions in Organo-Catalysis* at Emerging Trends in Chemical Sciences-2024 organized by University of Calcutta, February 2024.

16. Invited talk on *Computational Mechanistic Insights on Homogeneous Water Oxidation Versus Catalyst Deactivation* at

International Conference on Emerging Trends in Catalysis and Synthesis organized by IIT Kharagpur, March 2024.
17. Invited talk on *Harnessing Non-covalent Interactions in Catalysis* at Department of Chemical Sciences Meet organized by IISER Berhampur, March 2024.
18. Invited talk *on Computational Insights on Small Molecule Activation: A Case Study with 3d Transition Metal Catalyzed Water Oxidation* organized by IIT Bombay, IIT Kanpur and IISER Kolkata at Agra, July 2024.
19. Invited talk on *3d Transition Metal Catalyzed Water Oxidation: Computational Insights on Reaction Mechanism and Design of New Catalysts* organized by American Chemical Society, INSA and IIT Delhi at IIT Delhi, July 2024.

Workshops Attended

1. Materials Simulation Theory and Numerics organized by the International Centre for Theoretical Physics, Trieste, Italy held at IISER, Pune, July 2014.
2. Workshop on Electronic Structure, Atomistic and Statistical Modeling in Chemistry, Materials and Life Sciences, Organized by Schrödinger Materials at IACS, Kolkata, October 2014.
3. Chemical Science Symposium 2020: How can machine learning and autonomy accelerate chemistry? September 2020

Conference Session-Coordinator

1. National Conference on Graphene and Functional Materials (NCGFM-2018), CSIR – CMERI, February 2018.
2. Emerging Frontiers in Supply Chain Management, ICT-IOC Bhubaneswar, September 2019.
3. ChemCareers and One-Day Symposium on Young Talent in Chemical Sciences, Bhubaneswar, November 2019.
4. Five-Day Online Faculty Development Program on Recent Advancement in Chemical Biology and Drug Discovery, September 2020.
5. Virtual Integration of Synthesis with Theory and AI (online), July 2021.
6. DAE-BRNS National Workshop on Atomistic Modeling of Molecules and Materials (AMMM-2023), December 2023.
7. International Conference for Functional Materials and Polymer Technology (ICFMPT-2024), March 2024.

Academic Activities

Reviewer for Journal of the American Chemical Society, Nature Catalysis, Nature Communications, Angewandte Chemie International Edition, ACS Catalysis, Chemical Science, Chemical Engineering Journal, Green Chemistry, Catalysis Science and Technology, Organic Letters, Journal of Organic Chemistry, ChemCatChem, Chemistry - A European Journal, Langmuir, Biomacromolecules, European Journal of Organic Chemistry, Organic and Biomolecular Chemistry, RSC Advances, ChemPhysChem, ChemPlusChem, ChemistrySelect etc.

Editorial Advisory Board: ChemPlusChem (Jan 2021- Present); ChemPhysChem (Jan 2023 – Present)

Guest Editor and Initiator: Special Collection on Computational Chemistry to Study Organo-Catalytic Reaction Mechanisms by ChemPlusChem

Guest Editor: Special Collection on “Non-Noble Metal Catalysis” by ChemPhysChem

Presented personal views on **ChemPlusChem's 10th Anniversary Editorial**

Participated in an interview related to **improvement of the corporate website of Royal Society of Chemistry (rsc.org)** and experience in publishing with them.

Administrative Responsibilities

Past: Head Warden, Girls’ Hostel; Chair, Women Cell; Coordinator, Exam Committee; Member, Purchase Committee; Member, Library Committee; Member, Admission Committee; etc.

Sponsored Projects

1. CSIR ASPIRE Grant
2. SERB POWER Grant
3. INSPIRE Faculty Research Grant – DST
4. Institute Start-up Grant – ICT IOCB
5. MOE-STARS Research Grant (Co-PI)