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## Dr. Lisa Roy

Assistant Professor Grade I (Chemistry)  
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[Google Scholar](#)  
[ResearchGate](#)

[ORCID](#)  
[LinkedIn](#)

[Personal Homepage](#)  
[X \(Formerly Twitter\)](#)

### Educational Qualification

- **Ph.D(Science) in Chemistry (awarded in June 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. *Honored for excellence in B.Sc examination*.

### Professional Experience

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

- Associate Editor, International Journal of Quantum Chemistry, Wiley, January 2026 onwards
- Early Career Researcher (ECR) Editorial Board of Wiley Polymer Journals, January 2026 onwards
- DFG funded invitation to the international meeting, BioOxCat, at Bielefeld University, Germany, 2025
- Thieme Chemistry Journals Awardee, 2025
- Jury Member for Chemistry Europe Award Committee (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), since Jan2023
- SERB POWER (Promoting Opportunities for Women in Exploratory Research) Grant, 2021
- Early Career Advisory Board Member of *ChemPlusChem* (Chemistry Europe Society, Wiley VcH), since Jan2021
- 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 48<sup>th</sup> STC held at KIT in Germany
- Qualified the Graduate Aptitude Test in Engineering in 2010
- Qualified the 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 subtopics:

- 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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> and HCOO<sup>-</sup> 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<sub>2</sub> 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- $\pi$ -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<sub>2</sub> 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<sub>2</sub> Conversion*

**Lisa Roy**, Bhaskar Mondal and Shengfa Ye, **Dalton Trans.** 2020, 49, 16608 – 16616.

20. *Computational Investigation of the Mechanism of FLP Catalyzed H<sub>2</sub> 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<sub>sp</sub>-C<sub>sp</sub> 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- $\pi$ -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. (**Special Collection on Celebrating the 25th Anniversary of the Chemical Research Society in India**)

28. *The Role of Copper Salts and O<sub>2</sub> in the Mechanism of C $\equiv$ 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  $\alpha$ -Amino Acid Precursors Using Allylboronic Acids*

Samrat Sahu, Ganesh Karan, **Lisa Roy**, Modhu Sudan Maji\*, **Chem. Sci.** 2022, 13, 2355 – 2362.

30. *Solvophobicity-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<sup>3</sup>)-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 Zn<sup>2+</sup> 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. *Silylation 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,<sup>‡</sup> Sourav Bhunya,<sup>‡</sup> Asim Kumar Ghosh, Biswajit Sarkar, **Lisa Roy**, and Alakananda Hajra (<sup>‡</sup> 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,<sup>‡</sup> Subarna Pan,<sup>‡</sup> Arnadeep Datta, **Lisa Roy**\*, and Rajarshi Samanta\* (<sup>‡</sup> 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, 25, e202400533. **(Invited, for Board Members Special Issue)**

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, 26, 6760–6765

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.*, 2024,15, 14287-14294.

54. Overriding Cage Effect in Electron Donor-Acceptor Photoactivation of Diaryliodonium Reagents: Synthesis of Chalcogenides

Prahallad Meher, Sushanta Kumar Parida, Sanat Kumar Mahapatra, **Lisa Roy\***, and Sandip Murarka\* *Chem. Eur. J.* 2024, 30, e202402969. **(Cover Feature)**

55. BINAP-CuH-catalysed enantioselective allylation using alkoxyallenes to access 1,2-syn-tert,sec-diols

N. Navaneetha, Sundaram Maurya, Prativa Behera, Sandip B. Jadhav, Lakshmi Revati Magham, Jagadeesh Babu Nanubolu, **Lisa Roy\***, Rambabu Chegondi\* *Chem. Sci.*, 2024,15, 20379-20387

56. Ru(II)-Catalyzed [1,4]-Sigmatropic Rearrangement and Intramolecular Concerted SNAr of Aryl and Heteroarylthio Derivatives using Quinoid Carbene

Subarna Pan, Md. Saimuddin Sk., Bortika Sanyal, **Lisa Roy**, Rajarshi Samanta\* *ACS Cat.* 2024, 14, 18419–18428.

57. Enantioselective Synthesis of  $\alpha$ -Hydroxy Allyl Ketones via BINAP-CuH-Catalyzed Hydroacylation

Sundaram Maurya, N. Navaneetha, Prativa Behera, Jagadeesh Babu Nanubolu, **Lisa Roy\***, Rambabu Chegondi\*, *Angew. Chem. Int. Ed.* 2025, 64, e202420106.

58. Pallada-electrocatalysis enables distal regioselective and atroposelective olefination reactions

Subir Panja, Avishek Pan, Swastik Biswas, Chandan Das, Aritra Guha, Roshan Y. Nimje, T. G. Murali Dhar, Anuradha Gupta, Arvind Mathur, Arnab Datta\*, **Lisa Roy\***, Debabrata Maiti\* *Angew Chem. Int. Ed.* 2025, 64, e202422876.

59. Copper-Catalyzed Carbogermylation of Electron-Deficient Alkenes via 3,4- Difunctionalization of Quinoxalin-2(1H)-ones: Mechanistic Insights from Computational Studies

Asim Kumar Ghosh, Amit Mondal, Sukanya Neogi, Frenki Mahato, Sourav Bhunya, **Lisa Roy**, Alakananda Hajra\* *Chem. Eur. J.* 2025, 31, e202404186.

60. Minimal Catalytic Dissipative Assemblies via Cooperation of Amino acid, Nucleobase precursor and Cofactor

Syed Pavel Afrose, Soumili Roy, Pratip Bhattacharya, Ajeet Kumar Singh, **Lisa Roy** and Dibyendu Das\*, *Chem. Sci.* 2025, 16, 7838-7846.

61. Chelating-Group-Assisted C(sp<sup>2</sup>)-O Reductive Elimination at the Gold(III) Center

Avishek Das, Shivanshu Tripathi, **Lisa Roy\*** and Nitin T Patil\* *Org. Lett.* 2025, 27, 4853–4858

62. Non-equilibrium autopoietic vesicles driven by intrinsic catalysis

Sangham Jha, Soumili Roy, Antara Reja, Ajeet Kumar Singh, **Lisa Roy** and Dibyendu Das\*, *Chem (A Cell Press Journal)*, 2025, DOI: 10.1016/j.chempr.2025.102630

63. Merging Photochemical Olefin Metathesis with an Amination Reaction

Biprajit Paul, Surajit Das, Sanat Kumar Mahapatra, **Lisa Roy\*** and Indranil Chatterjee\*, *ACS Catalysis*, 2025, 15, 13810–13820

64. Silicon-Assisted Photocatalyzed C–O Bond Cleavage: Broader Applications and Mechanistic Investigations

Tanumoy Mandal, Sanat Kumar Mahapatra, Malekul Islam, **Lisa Roy\*** and Suman De Sarkar\*, *Org. Lett.*, 2025, 27, 9148–9154

65. Asymmetric Charge Injection Barrier Yields High Rectification in Rhenium(I)-Organometallic Compound

Subas Rajbangshi, Nila Pal, Ritu Gupta, Robinur Rahman, Pradeep Sachan, Vladimir Nesterov, **Lisa Roy**, Shishir Ghosh, Michael Zharnikov and Prakash Chandra Mondal, *J. Mater. Chem. C*, 2025,13, 20074-20084

66. Harnessing Selectivity and Reactivity with Non-Covalent Interactions in Molecular and Supramolecular Organo-Catalysis: A Computational Perspective  
Sanat Kumar Mahapatra, Bijoy Ghosh and **Lisa Roy\***, *ChemCatChem* 2025, 17, e01069 (*Invited for Special Collection on Women in Catalysis 2024*)
67. *Electron Donor-Acceptor Complex Offers a Diverse Approach for Carbonyl Alkylative Amination*  
Hrishikesh Paul, Arijit Chakraborty, Animesh Mandal, Dibyangshu Das, Sanat Kumar Mahapatra, **Lisa Roy\*** and Indranil Chatterjee\*, *Chem. Sci.* 2025, 16, 20061-20072.
68. Accessing Triplet State via Enhanced Intersystem Crossing in Covalent Organic Frameworks for Natural Sunlight-Driven Photocatalysis  
Amitha Agnes Fernandes, Ajeet Kumar Singh, Sk. Jubeda Begum, Sunny Sarkar, Varadharajan E., Santu Ruidas, Anita Das, Astam K. Patra, **Lisa Roy\***, Asim Bhaumik, Sasanka Dalapati\*, *ChemSusChem* 2026 (DOI: [10.1002/cssc.202502392](https://doi.org/10.1002/cssc.202502392))
69. Unveiling the Role of a Supramolecular Water Assisted Coupling of Pyrroles and Isocyanates to Amidopyrroles  
Sanat Kumar Mahapatra, Bijoy Ghosh and **Lisa Roy\***, *Phys. Chem. Chem. Phys.* 2026, (DOI: [10.1039/D5CP01713K](https://doi.org/10.1039/D5CP01713K)) (*Invited as part of themed collection: Advances in computational chemistry and catalysis*)
70. Late-Stage N-Me Selective Alkenylation and Alkynylation of Drugs and Unactivated Tertiary Amines Using Photoredox Catalysis  
Swagata Paul, Somenath Mahato, Sanat Kumar Mahapatra, Saitosh Mohanty, Sarani Dey, Suparna Mondal, Arpan Naskar, Srinivasa Srikar, Boudhayan Bandyopadhyay, Abhijit Das, **Lisa Roy\*** and Santanu Panda\*, *Nature Commun.* 2026 (10.1038/s41467-026-69131-7)

#### Book Chapter:

1. *Theoretical Approach to Homogeneous Catalytic Reduction of CO<sub>2</sub>: 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

##### (1) IIT KGP

###### M.Tech/PhD coursework

(CD61203) *Essential Tools for Scientific Computing: Basics of Unix, Bash Script programming.*

###### • B.Sc. Chemistry (Major)

**2025 Autumn Semester: (SD31215)** *Molecular Structure, Bonding And Spectroscopy: Quantum Mechanics and Chemical Bonding*

(SD21203) *Chemistry of Elements And Solid State: Reactions Kinetics and Mechanisms of Organometallic Complexes*

(SD29201) *Organic Chemistry Lab: Elemental Detection, Functional Group Identification, Synthesis.*

**2025 and 2026 Spring Semester: (SD11004)** *Introduction to Organic Chemistry: MO Theory, Electrophilic & Nucleophilic substitution reactions in aromatic systems, Reaction Profile.*

(SD11006) *Introduction to Physical Chemistry: The solid-state chemistry.*

(SD11022) *Chemical Thermodynamics and Kinetics: Chemical Kinetics.*

**2024 Autumn Semester: (SD21203)** *Inorganic Reaction Kinetics: Reactivity and stability of coordination compounds and their importance; labile and inert complexes, trans effect etc. Solid State Chemistry: Concept of lattices, packing, structures and defects in solids.*

##### (2) ICT-IOCB

###### • M.Sc. Chemistry

**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**

**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.*

- (3) **CSIR-CMERI**

- **PhD Coursework** undertaken at CSIR-CMERI for August 2018 session: Advanced Material Science

- (4) **MPI-CEC**

- **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 Sanat Kumar Mahapatra (PhD Research Scholar, ICT-IOCB), Prativa Behera (PhD Research Scholar, ICT-IOCB), Bijoy Ghosh (PhD research Scholar, IIT Kharagpur), Nupur Dutta (PhD research Scholar, IIT Kharagpur), Barnini Mukherjee (as Joint Supervisor, PhD research Scholar, IIT Kharagpur)
- Postdoctoral Research Fellow: Dr. Saurodeep Mandal
- Bachelor Thesis Project Student: Abha Mathur (BS-MS 4<sup>th</sup> Year Student, Chemistry Department, IIT Kharagpur)
- PhD Awarded at ICT Mumbai: Ajeet Kumar Singh (in June 2025), Thesis Title: ***Theoretical Approach to Investigate Water Splitting using Homogeneous Catalysts and its Applications***

## Invited 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<sub>2</sub> formation, CO<sub>2</sub> 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 16<sup>th</sup> 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 9<sup>th</sup> 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<sub>2</sub> 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<sub>2</sub>* 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. Keynote Lecture on *Catalysis in Computers: Mechanistic Insights for CO<sub>2</sub> 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 Faculty 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
12. 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.
13. 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.
14. Invited talk on *A Computational Perspective on Harnessing Non-covalent Interactions in Catalysis* at IIT Bombay, January 2024
15. 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.
16. 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.
17. 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.
18. Invited talk on *Harnessing Non-covalent Interactions in Catalysis* at Department of Chemical Sciences Meet organized by IISER Berhampur, March 2024.
19. Invited talk at ICOMC 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.
20. 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.
21. Invited talk on *Unravelling the Role of Non-Covalent Interactions and Confinement in Organo-/Supramolecular Catalysis* at Recent Advances in Chemical Sciences RACS-2024 held at IEST, Shibpur, November 2024.
22. Invited talk on *Computational Mechanistic Insights on the Role of Non-Covalent Interactions and Confinement Effects in Organo-/ Supramolecular Catalysis* at SoPhyC - Kolkata Chapter held at IISER Kolkata, December 2024.
23. Invited talk on *Computational Mechanistic Insights on the Role of Non-Covalent Interactions and Confinement Effects in Organo-/ Supramolecular Catalysis* at 7<sup>th</sup> International Conference on C-H Activation ISCHA – 7 held at IIT Bombay, December 2024.
24. Invited Lecture on *Computational Mechanistic Insights on Harnessing Bio-Inspired Oxidation Catalysis with Iron and other 3d Transition Metals* at the DFG-funded International Meeting on Bioinspired Oxidation Catalysis with Iron Complexes held at Bielefeld University, Germany, March 2025.
25. Web-based "ChemTalks" on Computational Interpretation of Selectivity and Reactivity in Organic Transformations organized by Thieme, India, June 2025.
26. Invited talk on *Theoretical Investigation of Water-Splitting using Homogeneous Transition Metal Complexes* at ACS-IACS Student Chapter, Symbiosis 2025, organized by IACS Kolkata, June 2025.
27. Invited Lecture on *Quantum Chemical Exploration of Regioselective, Enantioselective and Chemo-selective Organic Transformations: A Density Functional Theory Approach* at BBRC (Biocon Research Park), Bengaluru, September 2025.
28. Invited talk on *Theoretical Investigation of the Factors Governing the Reactivity in Molecular, Supramolecular and Enzymatic Transformations: A Density Functional Theory Approach*, at Recent Advances in Chemistry 2025, NIT Meghalaya, October 2025.
29. Invited talk on *Theoretical Investigations of Molecular, Supramolecular and Enzyme Catalyzed Organic Transformations: A Density Functional Theory Approach*, at ChemSpirit, IIT Hyderabad, November 2025

## Academic Activities

**Associate Editor:** International Journal of Quantum Chemistry (Jan 2026 – Present)

**Editorial Advisory Board:** ChemPlusChem (Jan 2021- Present), Presented personal views on ChemPlusChem's 10th Anniversary Editorial; ChemPhysChem (Jan 2023 – Present), Wiley Polymer Journals (Jan 2026 – Present)

**Guest Editor:** Special Collection on [\*From Computer to Bench and Back: in silico Elucidation of Organocatalytic Reaction Mechanisms\*](#) by ChemPlusChem

**Reviewer for** Journal of the American Chemical Society, Nature Catalysis, Nature Communications, Nature Synthesis, Angewandte Chemie, ACS Catalysis, Chemical Science, etc.

### **Administrative Responsibilities**

Present (at IIT Kharagpur): (Institute Level) Assistant Warden Savitri Bai Phule Hall 2; (Department Level) Professor-in-charge of Software Lab and Library, Co-coordinator of Research Committee, Member Purchase Committee

Past (at ICT-IOCB): Head Warden, Girls' Hostel; Chair, Women Cell; Coordinator, Exam Committee; Member, Purchase Committee; Member, Library Committee; Member, Admission Committee; etc.

### **Sponsored Projects (as PI)**

1. ANRF-ARG Grant, Recommended at IIT Kharagpur
2. IIT Kharagpur Faculty Start-up Research Grant, since July 2025
3. CSIR ASPIRE Grant: Ongoing at IIT Kharagpur, since October 2024
4. SERB POWER Grant: Completed at ICT-IOCB (June 2021-June 2024)
5. DST INSPIRE Faculty Research Grant: Completed at ICT-IOCB (October 2017 – October 2022)
6. Institute Start-up Grant – ICT IOCB, Completed (January 2020 – December 2021)