Arunava Sengupta

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# EDUCATION

*Research Experience: Post-Doctoral Work (2022-2025): Indian Institute of Technology (ISM) Dhanbad, Dhanbad, India (17 months).*

*Ph. D. (2011 - 2019) :* from Indian Institute of Technology Kanpur, Kanpur, India

Thesis Supervisor: Prof. Rabindranath Mukherjee.

Thesis Title: Coordination Chemistry of Transition Metal complexes with Tri-, Tetra- and Penta- dentate Pyridine/Pyrazine Amide Ligand (submitted May 2018).

Keywords: Coordination chemistry of 3d transition metal complexes, amide chemistry, C-H activation, fluorescence, kinetics, low-temperature spectroscopic analysis, EPR, Magnetism, DFT and TD-DFT studies.

*M. Sc. in Chemistry (2009 - 11):* from [University](http://www.iitkgp.ac.in/departments/home.php?deptcode=MP) of Calcutta (Rajabazar Science College Campus), Kolkata, India

Marks obtained: 733 / 1000

*B. Sc. in Chemistry (2006 - 09):* from [University of Calcutta (Raja Peary Mohan College, Uttarpara), India](http://www.jaduniv.edu.in/view_department.php?deptid=80).

First class with honours in Chemistry. Marks obtained: 68.87%

# RESEARCH

## Summary

In Ph.D. I have worked in the broad area of coordination chemistry of 3d-transition metals with pyridine/pyrazine-based amide ligands. During my PhD tenure, in particular, I have explored to what extent the physical and chemical properties of some of the biologically important metalloenzymes like bleomycin by biomimicking the enzymatic cores and replicating them with transition metal complexes. The characterization and deep understanding using various spectroscopic tools, like EPR, UV-Vis, Magnetism, cyclic voltammetry, and theoretical modeling with the help of DFT and TD-DFT studies. Two of the major themes of my research were (a) synthesizing coordination complexes of 3d-transition metal complexes of low and high oxidation states and (b) thorough analysis of their chemical properties with spectroscopic and theoretical analysis.

During the post-doctoral research project, I worked on photo redox catalysis and electro-organic synthesis for developing C-C andC-X bond formation. I also worked on developing carbohydrate-based 3d-transition metal chiral catalysts for asymmetric syntheses and reaction mechanism studies on C-H functionalizations using DFT studies.

*Research Projects*

1. Visible light offers an energy-efficient option for triggering chemical reactions. I used visible light for conducting reactions either through photo redox catalysis or catalyst-free pathways through the formation of ground-state donor-acceptor complexes for the formation of C-X bonds. (Chem. Commun. 2023, 59, 7455-7458, J. Org. Chem. 2023, 88, 6058-6070).
2. Sugar building blocks have traditionally been widely used for chiral pool-based synthetic strategies. However, their use for the development of chiral catalysts has been relatively less explored. As part of nature’s repertoire of chiral molecules, one of the drawbacks of designing sugar-based chiral organocatalysts or organometallic catalysts is that they are available in nature as only one enantiomer, thereby restricting their general wide applications. As part of my work in the area of carbohydrate-based chiral 3d-transition metal catalyst synthesis, I am involved in designing and developing carbohydrate-based ligands and organocatalysts that will be available in both their enantiomeric forms. (Catal. Sci. Tech. 2024, Manuscript under revision).
3. The fundamental nature of chemical reactivity involves the redistribution of electrons, and what can be better at moving them around than electricity? This energy-efficient method for conducting organic synthesis has motivated me to explore this method for developing C-C and C-X bond formation reactions, especially fluorination reactions. (ongoing project).
4. Detailed mechanistic studies on reaction mechanisms on C-H functionalization reactions by DFT calculations. (Ref. 1-22).
5. 3d-transition metal coordination complex formation with designed pyridine/pyrazine based amide ligands. (Ref-1, 20). Redox-chemistry and stabilization of metal-ligand radical in semiquinone form in the coordination complexes.

## Published or Accepted Papers

1. *T. Roy, K. Mondal, P. Halder,* ***A. Sengupta****, P. Das, “CuF2/DTBP-Catalyzed Chan-Lam Coupling of Oxazolidinones with Arylboronic Acid Pinacol Ester: Scope and Application” The J. Org. Chem.* ***2025****, ASAP article.*
2. *D. Paul, P. Sahoo,* ***A. Sengupta\*****, U. Tripathy\*, S. Chatterjee\*, “Revealing the Role of Electronic Effect to Modulate the Photophysics and Z-Scan Responses of o-Locked GFP Chromophores” 2025, The J. Phys. Chem. B.* ***2025****, 129(2), 692-711. (Selected as Cover Page Article).*
3. ***A. Sengupta****, S. N. Pandey, R. Bera, S. Ali, S. Yadav, “A sugar-derived ligand for room temperature aerial oxidation or non-aqueous Markovnikov hydration of styrenes via a preformed or in situ generated Co complex” Catal. Sci. Technol.* ***2024****, 14(16), 4487-4495. (Selected as Back Cover).*
4. *S. Bhowmik,* ***A. Sengupta****, R. N. Mukherjee, “Ni (ii) and Pd (ii) complexes of a new redox-active pentadentate azo-appended 2-aminophenol ligand: Pd (ii)-assisted intraligand cyclization forms a phenoxazinyl ring.” Dalton Trans.* ***2024****, 53(33), 14046-14064.*
5. *S. N. Pandey, N. Pathak,* ***A. Sengupta\*,*** *S. Yadav\*, “Understanding the gelation properties of the fluorophenyl glycosides of arabinoside gelators: experimental and theoretical studies.: Soft Matter* ***2024****, 20(36), 7111-7116. (Selected as Back Cover)*
6. *N. Mukhopadhyaya,* ***A. Sengupta****, F. Lloret, R. Mukherjee, “Phenoxazinyl Zn(II) diradical complex formed via redox-driven cyclization of a 2-aminophenolbased N3O ligand. Isolation of the modified N3 ligand radical and its Ni(II) complex.” Dalton Trans.* ***2024****, 53, 6515-6519. (Post-Doctoral Work).*
7. *H. Arora, G. Choudhir,* ***A. Sengupta****, A. Sharma, S. Sharma, “Bioactive metabolites of licorice and thyme as potential inhibitors of Cox1 enzyme of phytopathogens of Capsicum annuum L.: In-silico approaches.” J. Biomol. Struct. Dyn.* ***2024****, ASAP,* [*https://doi.org/10.1080/07391102.2024.2303603*](https://doi.org/10.1080/07391102.2024.2303603)*. (Collaboration Work).*
8. ***A. Sengupta****, A. Paul, B. Sarkar, S. Yadav, “Acetoxy Group-Directed Regioselective C2 alkenylation of indoles via Pd-Ag Bimetallic Catalysis”. ASAP version. J. Org. Chem.* ***2023****, https://doi.org/10.1021/acs.joc.3c01442. (A. Paul and A. Sengupta contribute equally to this work, Post-Doctoral Work).*
9. *A. Paul,* ***A. Sengupta****, S. Yadav, “Visible-light driven acetoxylation and deoxygenation of indoles via electron donor-acceptor complexes.” Chem. Commun.* ***2023****, 59, 7455-7458. (Post-Doctoral Work).*
10. *A. Paul,* ***A. Sengupta****, S. Yadav, “Organophotoredox-Catalyzed Cross-Dehydrogenative Sulfonamidation of Indoles and Other Heterocycles.” J. Org. Chem.* ***2023****, 88, 9599-9614. (Feature article and Cover Page Selected. Post-Doctoral work).*
11. *T. Roy, K. Mondal,* ***A. Sengupta****, P. Das, “CuF2/MeOH-Catalyzed N3-Selective Chan-Lam Coupling of Hydantoins: Method and Mechanistic Insight.” J. Org. Chem.* ***2023****, 88, 6058-6070. (Post-Doctoral Work).*
12. K. *Mondal,* N. *Mukhopadhyay,* **A. *Sengupta****,* T. *Roy,* P. *Das,* “*Exploiting Coordination Behavior of 7-azaindole for Mechanistic Investigation of Chan-Lam Coupling and Application to 7-azaindole Based Pharmacophores.*” *Chem.-Eur. J.* ***2023****, 29, No. e2022037.* (Post-Doctoral Work).
13. I. Wani, S. Sk, A. Mal, **A. Sengupta**, M. K. Ghorai, “ Stereoselective Routes to Hexahydropyrroloindioles and Tetrahydropyrroloquinolines from Activated Aziridines and Electron Deficient 3H-indoles”, Org. Lett, **2022**, 24, 7867. (IIT Kanpur) (Cover Page Article) (Collaboration work).
14. A Ali, S Bhowmik, **A Sengupta**, N Mukhopadhyay, R Mukherjee “Controlled C–H bond activation leads to orthometalation and ring-hydroxylation in Ni (II) and Pd (II) complexes of a common tridentate azophenyl-salicylaldimine ligand”, Inorg. Chim. Acta, **2022**, 538, 120960. (IIT Kanpur) (PhD Work).

## N Mukhopadhyay, **A Sengupta**, AK Vijay, F Lloret, R Mukherjee “Ni (ii) complexes of a new tetradentate NN′ N′′ O picolinoyl-1, 2-phenylenediamide-phenolate redox-active ligand at different redox levels” Dalton Trans., **2022**, 51, 9017. (IIT Kanpur) (Phd Work).

## NP Pathak, **A Sengupta** and S Yadav **“**Structure–gelation property relationships of phenolic glycosides of pentose sugars: pH dependent controlled release of curcumin”,Mater. Adv., **2022**, 3, 3906. (IIT Kanpur) (Collaboration work).

## I Verma, N Mukhopadhyay, **A Sengupta**, R Mukherjee “Arylamination via ortho-fusion on an azo-appended pyridine carboxamide complex of copper (II)”, J. Organomet. Chem., **2021**, 956, 122121. (IIT Kanpur) (PhD work).

## A Ali, **A Sengupta**, F Lloret, R Mukherjee “Switchover from NiIIN2O2 to NiIIN2O2S2 coordination triggered by ligand redox of a hemilabile noninnocent 2-aminophenolate”, J. Chem. Sci., **2021**, 133 (4), 1. (IIT Kanpurr) (PhD Work).

## M Manda, H Arora, **A Sengupta**, S Kant, F Lloret, R Mukherjee “Dimeric Mn (II), Co (II), Ni (II) and Cu (II) complexes of a common carboxylate-appended (2-pyridyl) alkylamine ligand: structure, magnetism and DFT study” New J. Chem., **2021**, 45 (35), 16019. (IIT Kanpur) (PhD Work).

## B. Sk, M. Sarkar, K. Singh**, A. Sengupta**, A. Patra, “UV to NIR multistate electrochromism and electrofluorochromism in dibenzophenanzine-arylamine derivatives, Chem. Commun. **2021**, 57, 13590. (IIT Kanpur) (Collaboration Work)

## N. Mukherjee, **A Sengupta**, R Mukherjee “Five-coordinate [(L2)2CuII(X)] z+ (X= H2O, z= 2; X= N3−, SCN−, NO2−, MeCO2−, Cl−, Br−, z= 1; L2= 1-benzyl-[3-(2-pyridyl)] pyrazole) complexes: Structural index, EPR and redox potential correlations”, Inorg. Chim. Acta, **2020**, 513, 119899. (IIT Kanpur) (Collaboration Work)

## A Kumar, **A Sengupta**, S Demeshko, R Mukherjee “Structure, magnetism and reactivity of a {MnIII(μ–O)2MnIV}3+ core towards oxidation of phenols”, Polyhedron, **2019**, 172, 226. (IIT Kanpur) (PhD Work).

## V. Veeraswamy, G. Goswami, S. Mukherjee, K. Ghosh, ML Saha, **A. Sengupta**, M. K. Ghorai, “ Memory of Chirality concept in asymmetric intermolecular michael addition of a-amino ester enolates to enones and nitroalkenes”, J. Org. Chem. **2018**, 83, 1106. (IIT Kanpur) (Collaboration Work)

## A. Rajput, A. Kumar, **A. Sengupta**, P. Tyagi, H. Arora, “ Copper (II) dimers stabilized by bis(phenol) amine ligands: Theortical and experimental insights:, New, J. Chem. **2018**, 42, 12621. (IIT Kanpur) (Collaboration Work)

## A. De, **A Sengupta**, F Lloret, R Mukherjee “Chemical Fixation of Atmospheric CO2 by Copper(II) Complexes of a Tridentate N‐donor Ligand”. Zeitschrift für anorganische und allgemeine Chemie **2018**, 644 (14), 801. (IIT Kanpur) (PhD Work)

## P Mukherjee, A. Das, **A Sengupta**, P Sen “Bimolecular Photoinduced Electron Transfer in Static Quenching Regime: Illustration of Marcus Inversion in Micelle” J. Phys. Chem B, **2017**, 121 (7), 1610. (IIT Kanpur) (Collaboration Work)

## **A. Sengupta**, A. Rajput, S. K. Barman, R. N. Mukherjee, “Low-spin [MII(L)2] and [MIII(L)2]+ (M = Fe and Co) complexes of tridentate azo-containing pyridine/pyrazine amide ligands: structures, properties and redox potential correlations”, Dalton Trans. **2017**, 46, 11291. (IIT Kanpur) (PhD Work)

## A Ali, **A Sengupta** R Mukherjee “Palladium(II) Complexes of a redox-active o-aminophenolate based ONSN ligand, Proof-of-concept of hemiliability in reactivity with PPh3 providing ONNP and ONSP coordination” J. Ind. Chem. Soc., **2015**, 92, 1981. (IIT Kanpur) (PhD Work)

# TEACHING EXPERIENCES

Assistant Professor in the Department of Chemistry at Techno India University, West Bengal, from Feb 2019-November 2020. (21 months). Assistant to Research and Development, Techno India University, West Bengal.

Teaching Assistant (graded assignments) in Indian Institute of Technology Kanpur, Kanpur, India, for B.Tech in theory and lab courses.

# PARTICIPATION IN SCHOOLS AND CONFERENCES

International Conferences attended and Poster/Oral Presentation:

1. 59th Annual Convention of Chemists 2022 (ACC-2022) & International Conference on Recent Trends in Chemical Science 2022 (RTCS-2022), (IIT Dhanbad, 2022) Organized by Indian Chemical Society, Kolkata. Professor A. K. Dey Award for Outstanding Oral Presentation. December 16-18, 2022

2. Asian Coordination Chemistry Conference (ACCC-6, RACI 2017 Centenary Congress), (Melbourne, Australia), (July 23-28, 2017).

3. SABIC 2017: 5th Symposium on Advanced Biological Inorganic Chemistry, January 7-11, 2017, organized by TIFR and IACS, The Stadel, Kolkata.

Conferences attended/Poster presented:

1. “Aerial C-H bond activation and aromatic ring hydroxylation in CuII and CoIII complexes of Schiff base containing phenol-carboxamide ligand” (Poster presentation), Arunava Sengupta and Rabindranath Mukherjee, Asian Coordination Chemistry Conference (ACCC-6, RACI 2017 Centenary Congress), (Melbourne, Australia), (July 23-28, 2017).

2. “Azo-containing Pyridine/Pyrazine Carboxamide Ligands: Series of Six Coordinated FeIII/II and CoIII/II Complexes: Structures, Properties and Trend of E1/2 Values For MIII/MII Redox Process” (Poster presentation), Arunava Sengupta, Amit Rajput, Suman K. Barman and Rabindranath Mukherjee, SABIC 2017: 5th Symposium on Advanced Biological Inorganic Chemistry, January 7-11, 2017 , organized by TIFR and IACS, The Stadel, Kolkata.

3. “Mixed-Valent Bis(µ-oxo) Dimanganese(III, IV) Complexes with different ligands and reactivity and Phenolic Substrates” Akhilesh Kumar, Arunava Sengupta and Rabindranath Mukherjee, SABIC 2017: 5th Symposium on Advanced Biological Inorganic Chemistry, January 7-11, 2017 , organized by TIFR and IACS, The Stadel, Kolkata.

4. RSC – IIT Kanpur Symposium in Chemical Science, November 23, 2015, Department of Chemistry, IIT Kanpur.

5. Complex Chemical Systems, November 2 – 3, 2015, Department of Chemistry, IIT Kanpur.

6. National Symposium on Radiation and Photochemistry (NSRP-2015), March 9-11, 2015, Department of Chemistry, IIT Kanpur.

7. CHEMFEST-2014 (October 11, 2014) (An In-House Symposium of the Department of Chemistry, IIT Kanpur).

8. Dynamics of Complex Chemical and Biological System (DCCBS 14), February 13 – 15, 2014, Department of Chemistry, IIT Kanpur.

9. International Collaborative and Cooperative Chemistry Symposium (ICCCS), October 24 – 26, 2013, Department of Chemistry, IIT Kanpur.

10. CHEMFEST-2012 (September 1, 2012) (An In-House Symposium of the Department of Chemistry, IIT Kanpur).

11. Mini-symposium in honour of Prof. S. Sarkar, March 2, 2012, Department of Chemistry, IIT Kanpur.

12. Celebration of Chemistry (International Year of Chemistry 2011) @ IITK, Department of Chemistry IIT Kanpur, India (December 3-5 2011).

Workshops attended:

‘Workshop on Column Structure and Chemistry (Merck) and Mass Spectrometry (Agilent)’

November 2, 2015, Department of Chemistry, IIT Kanpur

# ACADEMIC ACHIEVEMENTS

1. Got 1st rank in Raja Peary Mohan College in B.Sc. in Chemistry. Got Tatyana Sedina Saha Memorial Endowment Scholarships as the best Chemistry Honours student of 2009.

2. Got a rank as the top student in the M.Sc. inorganic chemistry specialization at the University of Calcutta (University College of Science Campus) in 2011.

# NON-ACADEMIC INTEREST

[Pen sketching. You are welcome to take a look !!](https://plus.google.com/photos/110844402797640688185/albums/5457304891366192081)

# Expertise: Hands-on experience with

# 1. Design and synthesis of multi-step syntheses of organic chelating ligands and their reactions with a variety of metal ions to isolate complexes with interesting properties.

# 2. Hands on experience on synthetic inorganic chemistry research and expertise in a number of characterization techniques such as IR, UV-Vis-NIR, 1H & 13C NMR, TGA, EPR, Mössbauer, single-crystal X-ray structure determination, Powder XRD, Cyclic Voltammetry, Differential Pulse Voltammetry and Coulommetry, Spectroelectrochemistry, Glove Box technique.

# 3. Knowledge of Programs such as Origin 6.0, 2017, Office 2013, ChemDraw 8.0, single-crystal Structure-solving programs (SHELX, WinGX, SIR-97, PLATON, Olex2, XSEED and related programs like ORTEP, DIAMOND, Mercury), WinEPR-SimFonia.

# 4. Familiar with DFT calculations: geometry optimization, broken-symmetry formalism, evaluation of magnetic-exchange coupling constant for dinuclear systems, TD-DFT, EPR with both Gaussian and Orca.

# 2025

# Madhepura, India Dr. Arunava Sengupta