Chemistry Connect

January 2025 Vol 2 Issue 1

From the HOD's Desk

WELCOME BACK!

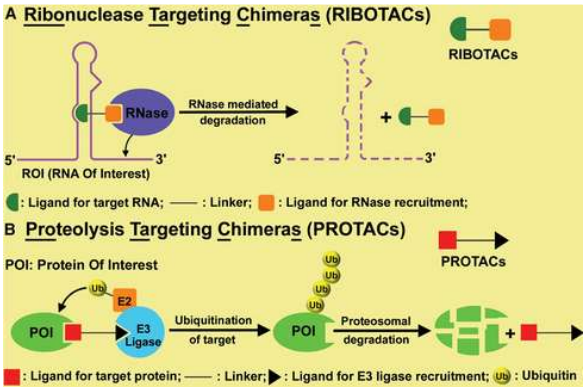
It is with great enthusiasm that I welcome you to the continuation of our departmental academic journey through our new newsletter, ***Chemistry Connect***. On behalf of the entire faculty, staff, and student body of the Department of Chemistry, I invite you to delve into the heart of our research and educational endeavors. This newsletter serves as a window into the vibrant world of discovery, collaboration, and innovation that defines our community. Our research leadership spans traditional areas such as physical, inorganic, organic, and analytical chemistry, while also expanding into emerging fields like chemical biology, environmental chemistry, biophysical chemistry, soft and hard materials chemistry, and nanotechnology. As the world faces evolving challenges—from healthcare and climate change to the integration of artificial intelligence, the depletion of natural resources, and the development of innovative materials—the landscape has changed dramatically over the past few decades. To address global challenges, we take a dynamic, adaptive approach, recognizing chemistry's crucial role in solutions. We are committed to advancing research, promoting inclusivity, and fostering a diverse environment for innovation. Our state-of-the-art undergraduate and postgraduate laboratories, supported by state funding, empower students to contribute to academic and translational progress.

We welcome your suggestions and feedback as we continue to elevate the Department to new heights. A big kudos to all our faculty and students for their dedication and hard work throughout our academic journey.

Warm regards,
Prof. Parthasarathi Das
Head of Department

Chemistry Buzz

In the previous issue of Chemistry Connect, we discussed about PROTACs (Proteolysis-targeting chimeras) which could selectively degrade disease causing proteins (Figure B). However, there are several human diseases that are caused by aberrant RNAs. To specifically degrade these disease causing RNAs, a novel type of molecules called Ribonuclease targeting chimeras (RIBOTACs) are being developed. RIBOTACs are bivalent molecules (Figure A) containing an RNA-binding module (green) and a ribonuclease (RNase) recruitment module (orange) joined by a linker (black line). Upon binding a target RNA, RIBOTACs recruit an RNase in close proximity of the target, thereby facilitating its degradation. This technology is pioneered by Dr. Mathew Disney at The Herbert Wertheim UF Scripps Institute, Florida, USA. Using this technology, RIBOTACs have been developed to target microRNAs involved in cancer and repeat containing RNAs in neurological disorders such as amyotrophic lateral sclerosis (ALS).



SPOTLIGHT

Dr. Sajal Kumar Giri

Department of Chemistry and Chemical Biology welcomes Dr. Sajal Kumar Giri, who recently joined as an assistant professor. He received his Ph.D. in 2020 from the Max Planck Institute for the Physics of Complex Systems in Dresden, Germany, under the guidance of Prof. J. M. Rost. His doctoral work is based on developing Machine Learning methods for applications in the area of molecular spectroscopy. Following his Ph.D., Dr. Giri conducted postdoctoral research in the group of Prof. George C. Schatz at Northwestern University, Evanston, USA, from 2021 to 2024. At IIT (ISM) Dhanbad, his future research will focus on AI-ML modeling for Chemistry.

Publications

1. Akhter, S. Sk.; Srivastava, D.; Mishra, A.; Patra, N.; Kumar, P.; **Padhi, S. K.***, Physicochemical Analysis of Cu(II)-Driven Electrochemical CO_2 Reduction and its Competition with Proton Reduction. *Chem. Eur. J.* **2024**, *30*, e202403321.
2. Mishra. A., and **Padhi, S. K.*** Harnessing Ruthenium and Copper Catalysts for Formate Dehydrogenase Reactions, *Chem. Rec.* **2024**, 24, e202400172. (Invited Article for the special issue on "Catalytic Transformation of Small Molecules")
3. Raj. M., and **Padhi, S. K.*** Decoding the Catalytic Potential of Dinuclear Ist-Row Transition Metal Complexes for Proton Reduction and Water Oxidation, *Chem. Rec.* **2025**, *25*, e202400170. (Invited Article for the special issue on "Catalytic Transformation of Small Molecules")
4. Enam, W.; Chowdhury, A.; Laichter, K.; Lin, K. L.; Mandal, A.; Malakar, B.; Bhaumik, A.; Muller, T. E.; **Chowdhury, B.***, Hydrodeoxygenation of Glycerol to Propene over Molybdenum and Niobium Phosphate Catalysts. *ChemCatChem* **2024**, *0*, e202401281.
5. Paul, D.; Sahoo, P.; Sengupta, A.; Tripathy, U.; **Chatterjee, S.***, Revealing the Role of Electronic Effect to Modulate the Photophysics and Z-Scan Responses of o-Locked GFP Chromophores. *J. Phys. Chem. B* **2025**, *129*, 2, 692−711.
6. Mondal, K.; Paul, S.; Halder, P.; Talukdar, V.; **Das, P.***, Iodine-Catalyzed Regioselective C-3 Chalcogenation of 7-Azaindoles: Access to Benzothiophene-Fused 7-Azaindole Analogs. *J. Org. Chem.* **2024**, *89*, 23, 17042−17058.
7. Bera, A.; Joshi, P.; **Patra, N.***, Delving into Macrolide Binding Affinities and Associated Structural Modulations in Erythromycin Esterase C: Insights into the Venus Flytrap Mechanism. *J. Chem. Inf. Model.* **2024**, *64*, 23, 8892−8908.
8. Srivastava, D.; **Patra, N.***, Improving the Computational Efficiency of the Adaptive Biasing Force Sampling by Leveraging the Telescopic-Solvation Scheme. *J. Chem. Theory Comput.* **2024**, *20*, 24, 10952−10960.
9. Kumar, M.; **Nayek, H. P.***, Organotin(IV) Compounds as Catalysts for the Solvent-Free Synthesis of Naphthofurans. *Organometallics* **2024**, *43*, 22, 2906−2915.
10. Pramanik, S.; Das, A. K.; Debnath, S.; **Maity, S.***, Introducing Alkyl Selenocyanates as Bifunctional Reagents in Photoredox Catalysis: Divergent Access to Ambident Isomers of −SeCN. *Org. Lett.* **2024**, *26*, 40, 8447-8452.
11. Hoque, I. U.; Debnath, S.; Lo, R.; **Maity, S.***, A chromatographic relay conjugated photoredox strategy: S, Se-pharmacophore from alkenes via formal [2+2+1] heteroannulation. *Chem. Commun.* **2024**, *60*, 12429-12432.
12. Kachhap, P.; **Haldar, C.***, Catalytic Oxidation of Aliphatic Alcohols by Hydrogen Peroxide Using Merrifield Resin-Supported Binuclear Dioxidovanadium(v) Complexes of Hydrazone Ligands as a Catalyst. *Top. Catal.* **2024**, *68*, 208-228.
13. Kachhap, P.; Chaudhary, N.; **Haldar, C.***, Impact of Surface Modification on the Oxidation of Linear Aliphatic Alcohols by Vanadium Complexes Supported on Merrifield Resin with Mixed Functionality Ligands. *ChemistrySelect* **2024**, *9*, 36, e202402642.
14. Pandit, Y. K.; Mahato, V.; **Udayabhanu, G.***, Titanium Dioxide Nanomaterial-Reinforced Particle Gel: Development, Characterization, and Performance Evaluation for Water Shutoff Jobs in Heterogeneous Reservoirs. *Energy Fuels* **2024**, *38*, 3, 1781−1798.
15. Pandit, Y. K.; Mahato, V.; **Udayabhanu, G.***; Ravishankar, B.; Dhandi, M., Preparation, Characterization, and Evaluation of a Nanomaterial Reinforced Particle Gel System for the Control of Excessive Water Production in Mature Oil Fields. *Geoenergy Sci. Eng.* **2024**, *235*, 212707.
16. Pandit, Y. K.; Kumar, A.; Mahato, V.; **Udayabhanu, G.***; Matey, S.*; Dhandi, M., Experimental Investigation of a Novel Alumina Nanomaterial Reinforced Particle Gel System for Water Shut-off Jobs in Heterogeneous Reservoirs: Fabrication, Characterization, and Performance Assessment. *Ind. Eng. Chem. Res.* **2024**, *63*, 36, 15665−15682.

Publications

17. Sen, T.; Biswas, A.; **Udayabhanu. G*.**; Thangavel, R.; Raut, T. K., Enhanced Electrochemical Performance of NiO Surfaces via Selective Li^+ Doping. *Phys. Chem. Chem. Phys.* **2024**, *26*, 27141-27151.
18. Maurya, A.; Pradhan, N.; Keshar, K.; Manisha; Yadav, M.*, Boron-Doped Fe_3S_4/Co_3S_4 Decorated with Multi-Wall Carbon Nanotubes as an Efficient Electrocatalyst for Oxygen Evolution Reaction in Alkaline Media. *J. Environ. Chem. Eng.* **2024**, *12*, 6, 114709.
19. Roy, R. K.; Sharma, M.; **Patra, N.***, SARS-CoV-2 Variants and Bebtelovimab: Immune Escape Mechanisms Revealed by Computational Studies. *Phys. Chem. Chem. Phys.* **2024**, *26*, 29929–29939.
20. Negi, K.; Kumar, A.; Chakraborty, G.; Sahoo, S.; Patra, S.; **Patra, N.**; Bhutia, S. K.; **Sahu, S. K.***, Rationally Designed Porous Self-Assembled Nanoparticles for Combinational Chemo-Photodynamic Therapy. *Dalton Trans.* **2024**, *53*, 17465-17479 (Published with Back Cover Page).
21. Roy, K.; Saha, A.; Saha, B.; Banerjee, S.; Mukhopadhyay, C.; **Sahu, S. K.**; Adak, L.*, Reusable Iron-Copper Catalyzed Cross-Coupling of Primary Amides with Aryl and Alkyl Halides: Access to N-Arylamides as Potential Antibacterial and Anticancer Agents. *Chem. Eur. J.* **2024**, e202403649.
22. Dey, S.*, Sahay, S. S., Rahaman, S., & Das, R. Iodine-Assisted Regioselective C3-H Chalcogenation of 4-Phenyl Aminocoumarin: Access to Unusual Dual Selenylation of N-Substituted Derivatives. *European Journal of Organic Chemistry*, **2025**, *28*, 4, e202401163.

Patents - filed & granted

1. Biswajit Chowdhury, Akash Surajlal Rane, and Aniruddha Singha filed IP application No. 202331045425 on 7th October 2024 for a catalyst for the synthesis of cyclic urea, a process for the preparation thereof.
2. Soumitra Maity filed IP application No. 202431083569 on 30th October 2024 for a novel bifunctional phosphoaminating agent, a process for the preparation thereof and the application thereof in the synthesis of aminophosphonates/aminophosphonic acids.
3. Kalipada Manna, Sagar Pal filed IP application No. 202431103949 on 28th December 2024 for a new light responsive polymeric micelle for real-time monitored delivery of therapeutics and a process for the preparation thereof.

Sponsored research projects sanctioned

Institute level International Academic cum Research program (in the scope of Indo-Norwegian Cooperation Program)
Title: Bioscopy - Towards modern transdisciplinary education and research in microscopy (Approved 20th Nov 2024); Funded by: H K Dir Norway and UGC (University Grants Commission) of India; Project No: INCP2-2024/10271; Co-PI: **Prof. Biswajit Chowdhury** (IIT-ISM) side; PI: Prof. Krishna Agarwal, Professor, UIT; The Arctic University of Norway

Invited Lectures

1. **Prof. S. K. Padhi** delivered an invited talk on “Evaluating Cu(II)-Catalyzed Electrochemical CO_2 Reduction: Insights into Proton Reduction Interference” in Morden Trends in Inorganic Chemistry (MTIC)-XXI, during 13th to 17th December 2024, organized by IIT Kharagpur.
2. **Prof. Soumitra Maity** delivered an invited talk on “A Photo Touch on Chalcogenonitriles: Harnessing Ambident Nucleophilicity by Light” at the National Symposium on Recent Advances in Chemical Sciences' (RACS-2024) during 7th to 9th November 2024 at IIEST, Shibpur.
3. **Prof. Parthasarathi Das** delivered an invited talk at the 7th International Symposium on C-H activation (ISCHA-7) during 6th to 9th December 2024 at IIT Bombay.
4. **Prof. Swapan Dey** delivered an invited talk on "Highly Fluorescent Boranil Materials and Their Applications as a Light Emitter" in RACS2024, during 7th -9th November 2024 at IIEST, Shibpur.

5. Prof. H. P. Nayek delivered invited talks on two distinct occasions: first, on "Organogermanium(IV) Catalysts for Organic Reactions" at the 21st International Conference on Modern Trends in Inorganic Chemistry (MTIC-XXI) held from December 14-17, 2024, at IIT Kharagpur, and second, on "Tetravalent Organogermanium/Tin Compounds as Catalysts for Organic Reactions" at the 7th International Conference on Frontiers in Chemical Sciences (FICS-2024) held from December 2-4, 2024, at IIT Guwahati.

6. Prof. Soumit Chatterjee presented an invited poster at the SoPhyC conference in October 2024 at IIT Bombay. He also delivered an invited talk at the prestigious international conference 'Optics Within Life Science (OWLS-17)' in November 2024, organized by TIFR, IIT Bombay, and the Fluorescence Society of India.

Prof. H.P. Nayek at 21st International Conference on Modern Trends in Inorganic Chemistry (MTIC-XXI) with his former supervisor Prof. Peter W. Roesky.

7. Prof. Sagar Pal delivered an invited talk on "Polymeric Gels and Micelles: An Overview from Synthesis to Applications" at the International Conference on Advances in Materials and Chemical Sciences (AMCS-24) from 18th -20th December 2024 at BIT, Mesra, Ranchi .

Prof. S.K. Padhi delivered invited lecture at the Morden Trends in Inorganic Chemistry (MTIC)-XXI organized by IIT Kharagpur.

Prof. H.P. Nayek at 7th International Conference on Frontiers in Chemical Sciences (FICS-2024)

Prof. Swapan Dey delivered an invited lecture at RACS2024, IIEST, Shibpur

Prof. Parthasarathi Das delivered invited lecture at ISCHA-7 at IIT Bombay

Events Organized

A two-day national workshop titled **"Green Steel Production via Decarbonization for Sustainable and Circular Economy (GSP2024)"** on 16th-17th December 2024 was organized by Dept. of CCB at IIT (ISM) Dhanbad with Prof. Madhulika Gupta (CCB) as Convenor and Prof. Ejaz Ahmad (Chemical Engineering) as Co-Convenor. GSP2024 was supported by the Department of Scientific and Industrial Research (DSIR), Anusandhan National Research Foundation (ANRF), Jharkhand Council on Science, Technology and Innovation (JCSTI), Council of Scientific and Industrial Research (CSIR), and Indian National Young Academy of Sciences (INYAS). The oral and poster prizes were sponsored by American Chemical Society (ACS) and Royal Society of Chemistry (RSC). GSP2024 had eminent speakers from AMNS, EIL, EY, HPCL, KBR, JSPL, SAIL Bokaro, TATA Steel, IIP, NABI, DST, IITs, CSIR labs and universities. About 240 industry leaders, researchers, policymakers, academicians and students from all over India joined GSP2024 to discuss the importance of decarbonization in steel production for meeting climate goals and promoting environmental stewardship.

Prof. Prem Vrat, Chairman, BoG, IIT(ISM) Dhanbad as Chief Guest for GSP2024. Prof. Sukumar Mishra, Director, IIT(ISM) Dhanbad; Prof. A.K. Mishra, Director, CSIR-CIMFR Dhanbad; and Prof. V. M. S. R. Murthy, Director, IIEST Shibpur as Guests of Honor for GSP2024. Prof. Parthasarathi Das, HoD, CCB as Chairman of GSP2024.

Vigyan Jyoti Program, Department of Science and Technology (DST)

Prof. Madhulika Gupta organized the third Vigyan Jyoti program on 25th November 2024 for over 51 students from JNV Jamtara, Jharkhand, to encourage young girls to pursue careers in STEM (Science, Technology, Engineering, and Mathematics) under the Vigyan Jyoti program of the DST, Government of India. Prof. Parthasarathi Das (HoD, CCB), Prof. Alok Das (Dean, IIE) and Prof. Sanjeev Sahu (M n C) discussed the advantages and life in STEM careers.
Robotics workshop was organized in JNV Koderma on 30th November 2024 under DST Vigyan Jyoti Program.

Group picture for DST Vigyan Jyoti Program

Innovation, Design, and Entrepreneurship (IDE) Boot Camp

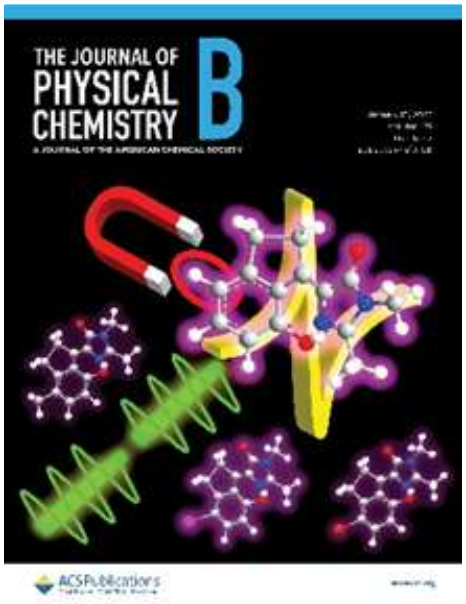
Prof. Madhulika Gupta and her students coordinated Two-Days Innovation, Design, and Entrepreneurship (IDE) Boot Camp for School Teachers of Jharkhand on 29 & 30 November 2024 under Innovation Cell, Ministry of Education, Government of India. This event was organized aiming to enhance the innovative and entrepreneurial skills of educators. The boot camp offered teachers hands-on activities, design thinking insights, and entrepreneurial strategies to enhance their teaching and foster creativity in students.

IDE Bootcamp

Other Achievements

- **Prof. S. K. Padhi** and collaborators showcase recent work in "Chem. Eur. J. 2024, 30, e202403321" DOI: 10.1002/chem.202403321 on the electrocatalytic reduction of CO_2 to CO, highlighting the use of Cu(II)-based molecular catalysts to achieve enhanced selectivity above 80%. They provide an in-depth explanation of their findings, which also reveal the concurrent generation of hydrogen (H_2) as a by-product during the CO_2 reduction process. This hydrogen evolution occurs through a competitive proton reduction reaction (HER), wherein two protons (H^+) are reduced by two electrons (e^-), leading to the formation of H_2. The study further explores the kinetic behavior of these reactions and uncovers a key mechanistic insight: the hydrogen evolution reaction (HER) proceeds prior to the CO_2 reduction reaction (CO_2 RR). This sequence of events suggests that HER, which competes for available electrons and protons, can significantly influence the efficiency and selectivity of CO_2 reduction. By examining the relative rates of the HER and CO_2 RR, the authors demonstrate that minimizing the rate of hydrogen production is critical for optimizing the yield of CO as the desired product. This work not only sheds light on the dynamics of proton and electron transfer during CO_2 reduction but also provides valuable insights into the competitive nature of the reactions occurring at the catalyst surface. Understanding these processes is crucial for designing more efficient catalysts that can selectively reduce CO_2 to CO while suppressing undesired by-products like hydrogen. The findings contribute to advancing the field of electrocatalysis and offer a clearer understanding of how to improve the performance of molecular catalysts in CO_2 reduction reactions.

- **Prof. Soumit Chatterjee's** work was featured on the Front Cover of the "The Journal of Physical Chemistry B" Volume 129, Issue 2, 2025.
- **Prof. Soumitra Maity's** work was featured on the Front Cover of the "Organic Letters" Volume 26, Issue 40, 2024. Alkylselenocyanates are introduced as bifunctional reagents for the simultaneous installation of alkyl groups and selenocyanate functionality onto alkenes. The cover takes inspiration from a galaxy, the astronomical centers of creation in the universe, where the addition of the alkylselenocyanate (on the right hand) and alkene (on the left hand) leads to their light-induced photo-fusion, creating selenocyanate-infused small molecules.



Prof. Soumit Chatterjee's work was featured on the Front Cover of the "The Journal of Physical Chemistry B"

Prof. Soumitra Maity's work was featured on the Front Cover of the "Organic Letters"

Students' Achievements

- Dr. Krishanu Mondal, from Prof. Parthasarathi Das' lab, has joined as a Postdoctoral researcher at the University of Tokyo, Japan.
- Dr. Sk Samim Akhter, from Prof. S. K. Padhi's lab, has received a Postdoctoral position from Kumoh National Institute of Technology, South Korea.
- Dr. Injamam Ul Hoque, from Prof. Soumitra Maity's lab, has joined as a Postdoctoral researcher at Hanyang University, Seoul, South Korea.
- Dr. Aparna Shukla, from Prof. Soumit Chatterjee's lab, has joined Ruhr-Universität Bochum, Germany, as a Humboldt postdoctoral fellow in November 2024.
- Dr. Dipankar, from Prof. Sagar Pal's lab, has joined as an Assistant Professor at NIPER Mohali, India.
- Dr. Abanindra, from Prof. Sagar Pal's lab, has joined as an Assistant Manager (R&D) at Black Rose Industries Ltd., India.
- Dr. Puja, from Prof. Sagar Pal's lab, has been awarded JSPS fellowship.
- Dr. Amit, from Prof. Sagar Pal's lab, has joined as a Senior Scientist in PACT, Cambridge, UK.
- Ashif Iqubal and Apurba Samanta delivered oral presentations, and Sachchida Nand Pandey and Segufa Rahaman presented a Poster at the XIX J-NOST Conference on 7th-9th Oct 2024 at IIT Gandhinagar.

Dr. Krishanu Mondal at University of Tokyo, Japan.

Sachchida Nand Pandey, Ashif Iqubal, Apurba Samanta, and Segufa Rahaman with Prof. Parthasarathi Das at IIT Gandhinagar.

- Gourav Chakraborty, Tripti Kundu, Partha Pratim Mondal, Ankit Joshi, (Ph.D. students), and Dr. Sarita Yadav (Postdoctoral Fellow) have won the Best Oral Presentation Awards and Vivek Semwal, Uday Bhan Yadav (Master's students) won the Best Poster Presentation Award at the GSP 2024 Workshop. The awards were sponsored by the American Chemical Society (ACS) and the Royal Society of Chemistry (RSC).


Awardees of the Best Oral and Poster Presentation at GSP2024 receiving their honors

- Reetika Tamang and Suprabha Palatasingh served as Jury Members for KALEIDOSCOPE24 at Dhanbad Public School (DPS) on 26th October 2024.


Ph.D. students Reetika and Suprabha at KALEIDOSCOPE24, DPS Dhanbad

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