

CHEMISTRY CONNECT



September 2024



Vol 1 Issue 1

Message from HoD's desk

Welcome!

It is with great avidity that I greet you to this new academic journey of the Department of Chemistry and Chemical Biology (CCB) as “Chemistry Connect”. On behalf of the faculty, staff and students of CCB, I invite you to explore our research and educational mission through this newsletter. Our leadership in research includes the traditional areas of physical, inorganic, organic and analytical chemistry, and has rapidly evolved to encompass chemical biology, environmental chemistry, drug discovery, biophysical chemistry, soft and hard materials chemistry, and nanotechnology. The rapidly changing world is facing newer challenges every day - from healthcare to climate change to incorporation of artificial intelligence to depleting natural resources to making new materials, today’s world is very different from what it was a few decades back. This warrants a constantly evolving approach in dealing with the changing times. Chemistry, being at the heart of many of these challenges, plays a particularly important role. We are committed to the advancement and inclusion of all students and aim to foster a diverse environment for academic and translational research. The modern research and UG-PG laboratories are equipped with state-of-art facilities along with the financial support from state funding agencies. Your suggestions and opinions are encouraged to promote the department to greater heights.

Kudos to all the faculties/students for their hard work throughout our academic journey.

Namaste!

Prof. Parthasarathi Das



Nobel Prize Winners 2024



David
Baker

Demis
Hassabis

John M.
Jumper

The Nobel Prize in Chemistry 2024 was awarded with one half to David Baker for “computational protein design” and the other half jointly to Demis Hassabis and John M. Jumper for “protein structure prediction”.



Victor Ambros

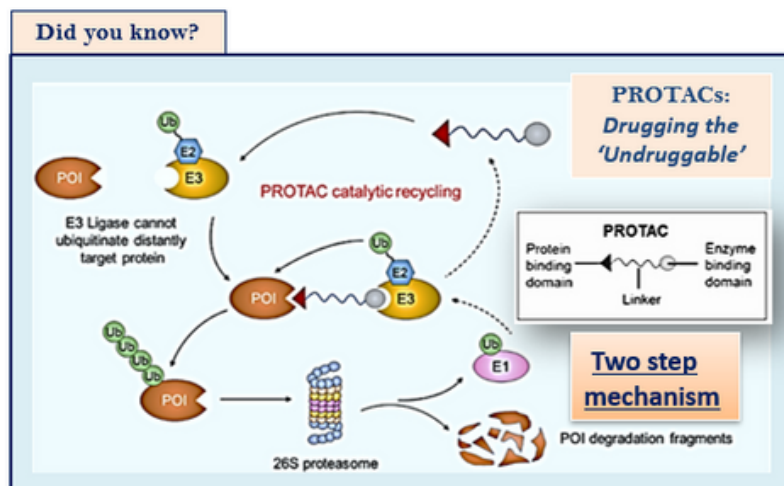


Gary Ruvkun

Victor Ambros and Gary Ruvkun have been jointly awarded the 2024 Nobel Prize in Physiology or Medicine “for the discovery of microRNA and its role in post-transcriptional gene regulation.”

Chemistry Buzz

PROTACs (Proteolysis-targeting chimeras) induced Targeted Protein Degradation (TPD) is now a novel therapeutic strategy in drug development, which degrade target protein by recruiting ubiquitin proteasome system. This emerging technology is employed in treating cancers, viral infections, immune disorders, and neurodegenerative diseases. e.g. ARV110 (androgen targeted PROTAC for prostate cancer).



Publications

1. Moon, P. R., Kujur, J. P., Kumar, A., & Pathak, D. D.* (2025). Mesoporous Co-doped-MgO as a new heterogeneous catalyst for the base-free synthesis of Quinoxalines. *Journal of Molecular Structure*, 1319, 139602.
2. Manna, K., Dolai, A., Ghosh, S., Samanta, S., Dey, S., & Pal, S.* (2024). Photoinduced Ultrafast Shape-Changing Self-Assembled Arylazopyrazole-Based Polymeric Micelles. *Macromolecules*, 57(17), 8445-8458.
3. Singha, K., Kumari, G., Jagadevan, S., Sarkar, A. N., & Pal, S.* (2024). In Situ Synthesis of Exfoliated Ni (OH)₂ Nanosheets and AgNPs-Embedded Functionalized Polyindole-Based Ternary Hybrid Microspheres: A Z-Scheme Photocatalyst for the Sunlight-Driven Degradation of Organic Pollutants with Enhanced Antibacterial Efficacy. *Langmuir*, 40(31), 16208-16225.
4. Manna, K., Roy, A., Dey, S., Kumar, A., & Pal, S.* (2024). Concentration-driven morphology change of a self-aggregated amino acid-inspired fluorescence-active copolymer for sustained release of hydrophobic drug. *Journal of Applied Polymer Science*, 141(39), e55991.
5. Das, D., Dey, S., & Pal, S.* (2024). Cytocompatible hydrogel derived from dextrin and Poly (N-Vinyl acetamide) toward controlled antimicrobial release. *Journal of Macromolecular Science, Part A*, 1-10.
6. Deb, M., Singh, H., Manhas, D., Nandi, U., Guru, S. K., & Das, P.* (2024). Development of di-arylated 1, 2, 4-triazole-based derivatives as therapeutic agents against breast cancer: synthesis and biological evaluation. *RSC Medicinal Chemistry*, 15(9), 3097-3113.
7. Halder, P., Mondal, K., Jash, A., & Das, P.* (2024). Exploiting Chloroform-CO₂ Chemistry for Pd-Catalyzed Carbonylation of Naturally Occurring and Medicinally Relevant Phenols, *The Journal of Organic Chemistry*, 89(13), 9275–9286.
8. Talukdar, V., Mondal, K., Halder, P., & Das, P.* (2024). Ullmann-Type N-, S-, and O- Arylation Using a Well-Defined 7-Azaindole-N-oxide (7-AINO)-Based Copper (II) Catalyst: Scope and Application to Drug Synthesis. *The Journal of Organic Chemistry*, 89(11), 7455-7471.
9. Kumar, M., & Nayek, H. P.* (2024). Syntheses and exploration of the catalytic activities of organotin (IV) compounds. *Dalton Transactions*, 53(23), 9827-9837.
10. Vinayak, R., Basu, D., Bhowmick, A., Ghosh, A., & Nayek, H. P.* (2024). Imine-functionalized organotin (IV) carboxylates: Syntheses, structures and antibacterial activities. *Inorganica Chimica Acta*, 568, 122093.
11. Rahaman, S., Sahay, S. S., Kumari, A., & Dey, S.* (2024). Multicomponent Cross-Dehydrogenative Coupling of Imidazo [1, 2-a] pyridine: Access to Abnormal Mannich and Mannich-Type Reaction. *The Journal of Organic Chemistry*, 89(15), 10773-10784.
12. Pandey, S. N., Pathak, N. P., Sengupta, A., & Yadav, S.* (2024). Understanding the gelation properties of the fluorophenyl glycosides of arabinoside gelators: experimental and theoretical studies. *Soft Matter*, 20(36), 7111-7121.
13. Kumar, A., Negi, K., & Sahu, S. K.* (2024). Gram-scale synthesis of aggregation-caused quenching-resistant red-emissive carbon dots for potential applications. *New Journal of Chemistry*, 48(16), 7265-7276.
14. Negi, K., Pathak, N. K., Tripathy, U., Dey, S. K., & Sahu, S. K.* (2024). Two-photon NIR-responsive carbon dots incorporated into NMOFs for targeted photodynamic therapy. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 694, 134163.
15. Mukherjee, P., Guha, S., Ghosh, A., Kar, K., Das, G., & Sahu, S. K.* (2024). Porous Organic Polymer-Based Nanocomposites for Hypoxia Relieving and Enhanced Chemotherapy in Hepatocellular Carcinoma. *ACS Applied Bio Materials*, 7(9), 6138-6151.
16. Mishra, A., Srivastava, D., Raj, D., Patra, N., & Padhi, S. K.* (2024). Formate dehydrogenase activity by a Cu (II)-based molecular catalyst and deciphering the mechanism using DFT studies. *Dalton Transactions*, 53(3), 1209-1220.
17. Pramanik, S., Samanta, A., & Maity, S.* (2024). A two carbon homologation of Friedel–Crafts alkylation enabled by photochemical alkene stitching: modular assembly of cyclolignans. *Chemical Communications*, 60(40), 5282-5285.
18. Hoque, I. U., Samanta, A., Pramanik, S., Chowdhury, S. R., Lo, R., & Maity, S.* (2024). Photocascade chemoselective controlling of ambident thio (seleno) cyanates with alkenes via catalyst modulation. *Nature Communications*, 15(1), 5739.
19. Pandey, S. N., Sengupta, A., Bera, R., Ali, S. & Yadav, S.* (2024). A sugar-derived ligand for room temperature aerial oxidation or non-aqueous Markovnikov hydration of styrenes using a preformed or in situ generated Co complex, *Catalysis Science and Technology*, 14(16), 4487-4495.

20. Srivastava, D., & Patra, N.* (2024). Elucidating Daptomycin's Antibacterial Efficacy: Insights into the Tripartite Complex with Lipid II and Phospholipids in Bacterial Septum Membrane. *The Journal of Physical Chemistry B*, 128(18), 4414-4427.
21. Bera, A., Mukherjee, S., & Patra, N.* (2024). Exploring the Transmembrane Allostery in MexB: DB08385 Variant as Promising Inhibitor like Candidate Against *Pseudomonas aeruginosa* Antibiotic Resistance—A Computational Study. *Physical Chemistry Chemical Physics*, 26(24), 17011-17027.
22. Naskar, A., Roy, R. K., Srivastava, D., & Patra, N.* (2024). Decoding Inhibitor Egression from Wild-Type and G2019S Mutant LRRK2 Kinase: Insights into Unbinding Mechanisms for Precision Drug Design in Parkinson's Disease. *The Journal of Physical Chemistry B*, 128(28), 6657-6669.
23. Chakraborty, G., & Patra, N.* (2024). Elucidating the Molecular Basis of 14–3–3 Interaction with α -Synuclein: Insights from Molecular Dynamics Simulations and the Design of a Novel Protein-Protein Interaction Inhibitor. *The Journal of Physical Chemistry B*, 128(29), 7068-7085.
24. Roy, R. K., Bera, A., & Patra, N.* (2024). Insights into Allosteric Inhibition of the AcrB Efflux Pump: Role of Distinct Binding Pockets, Protomer Preferences, and Crosstalk Disruption. *Journal of Chemical Information and Modeling*, 64(15), 5964-5976.
25. Shukla, A., Biswal, A. S., Chowdhury, A., Halder, R., & Chatterjee, S.* (2024). Aggregation-induced modulation of ground and excited state photophysics of 5- (tert-butyl)-2-hydroxy-1,3-isophthalaldehyde (5-tBHI). *The Journal of Physical Chemistry B*, 128(22), 5437–5453.
26. Kundu, T., Suyash, S., Gupta, M.,* & Chowdhury, B*. (2024). Introduction to greenhouse gases composition and characteristics in *Advances and Technology Development in Greenhouse Gases: Emission, Capture and Conversion* (pp. 3-18). Elsevier.

Patents - filed & granted

1. Abhay Shankar Patra, Priyapratim Patra, Sagar Pal, and Asim Kumar Mukherjee were granted Indian Patent No. 548923 on 28th August 2024 for their invention titled "Alginate acid/sodium alginate-based polymer as an organic binder in iron ore pelletization" (Application No. 202131014773, dated 31st March, 2021).
2. Biswajit Saha, Abhay Shankar Patra, Priyapratim Patra, Sagar Pal, and Asim Kumar Mukherjee were granted IP No. 532143 on 4th April 2024 for their invention titled "Carboxymethyl cellulose-based polymer as an organic binder in iron ore pelletization" (Application No. 202131014760, dated 31st March 2021).
3. Thillai Natarajan & Sumanta Kumar Padhi filed IP application No. 202431070872 on 19th September 2024 on catalyst for green hydrogen generation, a process for the preparation thereof, and the use thereof for green hydrogen generation from ammonia.
4. Aman Mishra & Sumanta Kumar Padhi filed IP application No. 202431048509 on 25th June 2024 on the process for the preparation of methanol by the hydrogenation of bicarbonate and carbon dioxide (CO₂) captured from air.
5. Aman Mishra & Sumanta Kumar Padhi filed IP application No. 202431048508 on 25th June 2024 on the process for the hydrogenation of carbon dioxide (CO₂) to methanol.

Sponsored research projects sanctioned

1. Title: Electrocatalytic and photo-electrocatalytic reduction of protons or carbon dioxide; Funding Agency: The Swedish Foundation for International Cooperation in Research and Higher Education (STINT); Type of Grant: Mobility Grants for Internationalisation: India programme; PIs: Prof. Ebbe Nordlander (Swedish PI) and Prof. Sumanta Kumar Padhi (Indian PI); Sanctioned Amount: SEK 190,000 Duration: October, 2024 to October 2027.
2. Title: Development of novel high-performance polymeric admixture for concrete and thereof; Sponsored by: JSW Cement Limited, Mumbai; Principal Investigator (PI): Prof. Sagar Pal; Sanctioned Amount: Rs. 15,75,300 Duration: 1st September 2024 to 31st December 2025.
3. Title: Effective utilization and life enhancement of tailing pond at West Bokaro; Sponsored by: Tata Steel Ltd., Jamshedpur; PI: Prof. Sagar Pal; Sanctioned Amount: Rs. 27,26,484; Duration: 1st June, 2024 to 30th September 2025.

Special Achievement

Prof. Madhulika Gupta was nominated by Anusandhan National Research Foundation (ANRF), Ministry of Science and Technology, Govt. of India among 20 women scientists working under AI, health care and energy solutions to represent India in the ASEAN-India Women Scientists Conclave (AIWSC) from 24th to 26th April 2024 in Singapore co-organized by Singapore's Agency of Science, Technology, and Research (A*Star) with India's Department of Science & Technology and ANRF with the support of the ASEAN Secretariat. The AIWSC included presentations on scientific achievements by women scientists, sharing sessions on overcoming societal expectations from women in STEM, panel discussions, and competition on innovation for selected participants on innovative projects within the scientific themes of the conclave. She was also selected among the 8 women scientists to be invited by High Commission India in Singapore with officials from DST to discuss research opportunities in Singapore on 27th April 2024.



Prof. Madhulika Gupta at ASEAN-India Women Scientists Conclave



Prof. Madhulika Gupta at High Commission India in Singapore



Group image of 20 women scientists representing India in AIWSC

Workshop Announcement

CCB is pleased to announce a two-day National Workshop on “Green Steel Production via Decarbonization for Sustainable and Circular Economy (GSP2024)” from 16th-17th December, 2024 at IIT(ISM) Dhanbad.

Visit <https://people.iitism.ac.in/~GSP2024/> or email gsp2024@iitism.ac.in for more details!

Invited Lectures

1. Prof. Biswajit Chowdhury delivered a lecture at Sun Petrochemicals Pvt Limited, Mumbai on 21st May, 2024. He also delivered a lecture in the National Conference on Catalysis for Energy, Environment and Sustainability (CEES-2024) at Indian Institute of Chemical Technology (IICT), Hyderabad during 18th to 20th September 2024.
2. Prof. Swapan Dey delivered a lecture on “One day International Seminar on Recent Advances in Chemical and Biological Sciences,” on 21st June 2024 at Alipurduar University, entitled, ‘Directed Molecular Recognition: Theory and its Potential Applications.
3. Prof. Hari Pada Nayek delivered a talk at 30th International Conference on Organometallic Chemistry during 14th to 18th July 2024 in Agra U.P.



Prof. Biswajit Chowdhury at CEES-2024

4. **Prof. Parthasarathi Das**, delivered lecture in 12th Asian Network for Natural and Unnatural Materials, at Department of Chemistry, IIT Bombay, from 20th to 22nd July 2024. He also delivered a talk in CRS Symposium 2024 – Rasayan 19 Science Beyond Boundary: Invention, Discovery, Innovation and Society, Department of Chemical Sciences, IISER Kolkata, from 29th to 30th July 2024.

5. **Prof. Soumitra Maity** conducted a refresher Course on Advanced Molecules and Materials for Sustainable Chemistry from 28th August 2024 to 10th September 2024 at UGC Malaviya Mission Teacher Training Centre, the University of North Bengal on “Photo-Redox Catalysis: Mimicking Nature’s Process for Sustainable Future”.

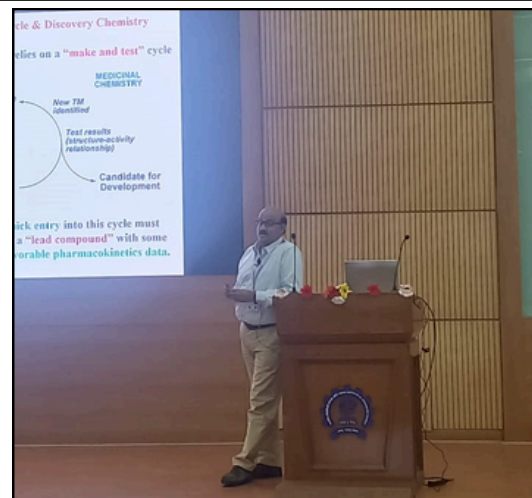
6. **Prof. Devendra Deo Pathak** delivered a Plenary Lecture on “Graphene Oxide-based 2D Nanocomposites as Versatile Heterogeneous Catalysts for Organic Synthesis” in Global Summit on “2D Materials and Graphene Technology (GS2DMAT2024)” on 17th September 2024 through Webinar.

7. **Prof. Sagar Pal** delivered a talk on “Biopolymeric Materials: From Development to Applications in Environmental Remediation” in AICTE-VAANI sponsored seminar on RA2M-SD 2024 from 7th to 9th August 2024 at HIT, Haldia on 8th August 2024.

He was also a chairperson of Technical Session 4, International Conference on Materials and Membranes for Water and Energy (ICMMWE-2024), CSMCRI, Bhavnagar, during 10th to 12th July 2024.

8. **Prof. Sumanta Kumar Padhi** visited LUND University from 12th June 2024 to 28th June 2024, Sweden under the STINT, INDIA Initiation Grant funded by “The Swedish Foundation for International Cooperation in Research and Higher Education (STINT)” in collaboration with Prof. Ebbe Nordlander. During the visit, the “Electrocatalytic proton and carbon dioxide reduction” using homogeneous catalysts was discussed and the output of the project was decided to be communicated in the international journal of repute. On 26th June 2024, Dr. Padhi delivered an invited talk on “Homogeneous Catalysts in activating HCOOH and CO₂” at the University of Southern Denmark (SDU), Odense, Denmark. The future collaborations on CO₂ reduction were discussed with Prof. Christine Joy Mckenzie, University of Southern Denmark (SDU).

9. **Prof. Madhulika Gupta** was invited for role model interaction at JNV Koderma to inspire students in STEM education on 09th September 2024. During her visit, she delivered an empowering role model talk. She shared insights into how programs like Vigyan Jyoti can help bridge the gender gap by providing the necessary support and resources for young women to excel in these domains.



Prof. Parthasarathi Das at IIT Bombay



Prof. Sumanta Kumar Padhi at Lund university



Prof. Sumanta Kumar Padhi at SDU

Events Organized

Yusuf Hamied Chemistry Camp

The Department of Chemistry and Chemical Biology (CCB) hosted the 60th Yusuf Hamied Chemistry Camp at IIT(ISM) Dhanbad from 7th to 9th June 2024, under the Royal Society of Chemistry’s Inspirational Science Programme. The Programme was supervised by Prof. Parthasarathi Das and Mrs. Melissa Mendonza, with the help of 12 research scholars. The camp engaged 77 students (39 girls and 38 boys) from 15 government schools in activities like laboratory experiments and scientific lectures. Participants received certificates and materials, including school bags, periodic table, T-shirts, and travel allowances, from the Yusuf Hamied Foundation.



Organizing team (on the left) and students (on the right) attending the 60th Yusuf Hamied Chemistry Camp

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

Prof. Madhulika Gupta organized a special one-day program on 20th August, 2024 for over 70 students from PM SHRI School Jawahar Navodaya Vidyalaya (JNV), Koderma, Jharkhand to encourage young girls to pursue careers in STEM (Science, Technology, Engineering, and Mathematics) under Vigyan Jyoti program of the DST, Government of India. Prof. Gupta organized a second event under this initiative for 61 female students from JNV Dhanbad on 3rd September, 2024. Prof. Dheeraj Kumar (Deputy Director), Prof. Sukha R. Samadder, (Associate Dean, R & D), Prof. Ejaz Ahmad (FIC, SRIC), Prof. Parthasarathi Das (HoD, CCB), Prof. Alok Das (Dean, IIE), and Prof. Sanjiv Sahu (MC) discussed the importance of STEM and under-representation of women in such careers.



Professors lighting the lamp during the inauguration ceremony



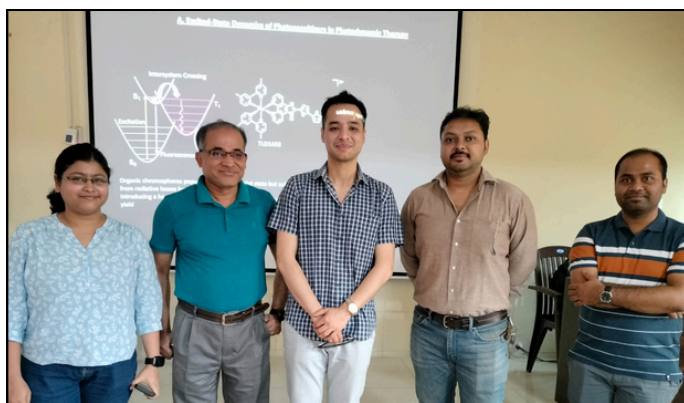
A glimpse into the treasured moments of the Vigyan Jyoti Scheme

Science fest

Prof. Naga Rajiv Lakkaniga's lab hosted an engaging science fest for local school children from 8th to 10th at the i2h building. The event aimed to spark curiosity and interest in science through a series of fun and interactive experiments and activities. Students explored various scientific concepts in physics, chemistry, and biology through the demonstration. The event was a success, encouraging them to pursue STEM education in the future.



Glimpses from the Science fest at i2h building



Guest Lecture by Dr. Avinash Chettri

Guest Lecture

Prof. Sumanta Kumar Padhi arranged a guest lecture by Dr. Avinash Chettri (Friedrich Schiller University, Germany), an alumnus of our department, who delivered an invited talk on the topic- "Unravelling the Excited-State Dynamics of Light-Responsive Materials with Time-Resolved Spectroscopy".

Other Achievements

- **Prof. Sagar Pal's** research group developed a biopolymeric reagent (TRL Level: 7) that has proven efficient as an organic binder in iron ore pelletization during plant trials. This work was part of a joint research project between Tata Steel Raw Materials Division and IIT(ISM) Dhanbad. A patent for this innovation has been granted (Patent No: 548923, Date of Grant: 28th August 2024).
- **Prof Sagar Pal's** work was featured on the Front Cover of Journal of Macromolecular Science, Part A: Pure and Applied Chemistry, Volume 61, Issue 6, 2024.
- **Prof Biswajit Chowdhury**, visited UIT, the Arctic University of Norway, Tromso from 10th June 2024 to 10th July 2024 as a visiting researcher where Prof. Krishna Agarwal was host faculty. During his stay, he discussed collaborative research between IIT (ISM) and UIT, master/doctoral student exchange through the Indo-Norwegian Cooperation Programme 2024, and a proposal was submitted.
- **Prof. Madhulika Gupta** was selected among 24 participants from the country for the Work & Industry Neutral Growth Skills Workshop (WINGS) 2024 Capacity Building Workshop organised by the Indian National Young Academy of Science (INYNAS) under its flagship event WiSDoM (Women in Scientific Domain) program at IIT Bombay from 8th to 10th August 2024. The WINGS Workshop is designed to empower future women leaders with prominent skills for professional escalation and leadership in both academia and industry.



Prof. Biswajit Chowdhury's visit to UIT



Prof. Sagar Pal's work on Cover page of J. Macromol. Sci., Part A

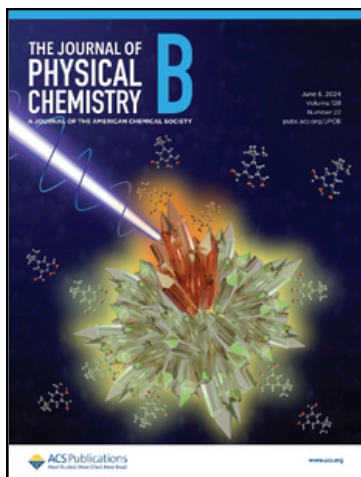
Students' Achievements

- **Dr. Aniruddha Singha** from Prof. Biswajit Chowdhury's lab joined as a Research Associate at Tata Steel Pvt. Limited, Jamshedpur.
- **Dr. Aman Mishra** from Prof. Sumanta Kumar Padhi's lab received a postdoctoral position at Lund University, Sweden.
- **Dr. Sarita Yadav, Tripti Kundu, Ankit Joshi, Suprabha Palatasingh, Reetika Tamang, Shariq Farhan Elaihi, Aakash Rajpoot, Vivek Semwal, and Uday Bhan** shared their academic experiences and inspired the students to consider advanced studies and careers in STEM with students from JNV Koderma and JNV Dhanbad under Vigyan Jyoti initiative of DST.

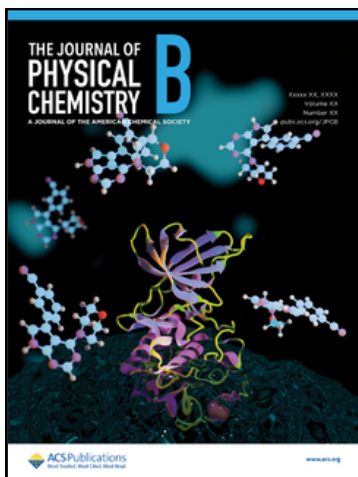


Ankit Joshi, Suprabha Palatasingh and Reetika Tamang from Prof. Madhulika Gupta's lab interacted with students of JNV Koderma to promote STEM education.

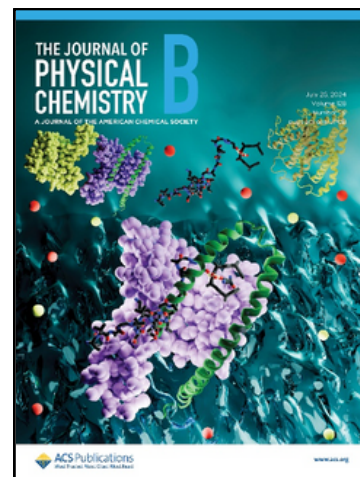
- Dr. Aparna Shukla from Prof. Soumit Chatterjee’s lab is joining Prof. Martina Havenith-Newen’s group as a Humboldt post-doc fellow.



Cover page designed by Dr. Aparna Shukla, PhD student of Prof. Soumit Chatterjee



Cover page designed by Avigyan Naskar, Rakesh K. Roy, Diship Srivastava, PhD students of Prof. Niladri Patra

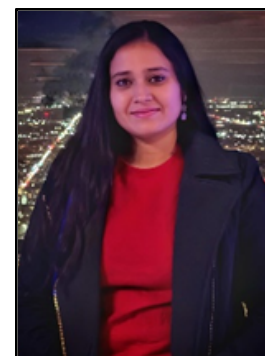


Cover page designed by Gourav Chakraborty, PhD student of Prof. Niladri Patra

Alumni Corner

Message from Dr. Arpita Roy, Post-Doctoral Research Fellow at UCLA

“I had the privilege of completing both my M.Sc. and Ph.D., supported by the DST-INSPIRE fellowship from CCB, IIT(ISM) Dhanbad. The department provided a strong foundation with excellent research facilities and a collaborative, supportive environment. I am deeply grateful to my Ph.D. supervisor, Prof. Sagar Pal, whose guidance and encouragement were invaluable throughout my research career. I have published 13 research articles, 4 review articles, received recognition at international conferences during my academic journey at CCB. I also received best Ph.D. Thesis award in the departmental and institutional level in the year 2022. The collaborative and friendly atmosphere, along with the state-of-the-art central research facility, significantly contributed to my achievements and paved the way for my current position.”



Dr. Arpita Roy from Prof Sagar Pal’s lab



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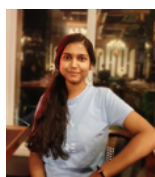
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