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# CHEMISTRY CONNECT

## IIT (ISM) DHANBAD

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## From the Head's Corner

We are pleased to present the third edition of *Chemistry Connect*, showcasing the achievements and activities of the Department of Chemistry and Chemical Biology at IIT (ISM) Dhanbad from July-September 2026.

This issue highlights the department's continued progress in research, featuring significant contributions across spectroscopy, photochemistry, organometallic chemistry, chemical biology, and materials chemistry. Research highlights include the development of environment-sensitive fluorescence probes for investigating protein conformational dynamics, a switchable synthetic strategy for pharmaceutically relevant spirocycles, the design of bifunctional organotin catalysts for efficient solvent-free hydroboration, and the development of high-efficiency lead-free chalcogenide perovskite solar cells through first-principles calculations, SCAPS-1D simulations, and machine learning. During this quarter, the department has made significant contributions to research through the publication of several high-quality research articles across diverse domains of Chemistry and Chemical Biology.

The progress in this quarter also witnessed vibrant academic engagement through inspiring research talks and invited lectures delivered by eminent scientists. Academic visits and outreach initiatives further strengthened our collaborative and interdisciplinary research environment.

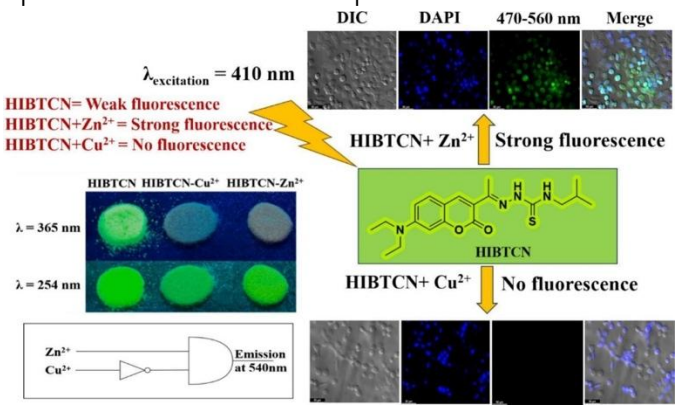
The Faculty and Student Spotlights reflect the broader impact of our academic community in nurturing talent, fostering innovation, and contributing to scientific advancements on a global scale.

As we look forward to upcoming events and new initiatives, the department remains committed to advancing excellence in research, education, and innovation. I extend my sincere appreciation to all faculty members, students, staff, and alumni for their dedication, enthusiasm, and invaluable contributions that continue to strengthen our academic community.

# Research Activity

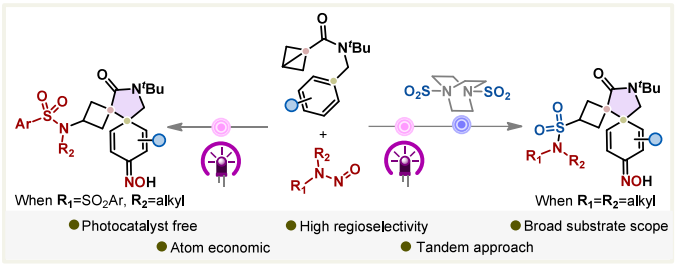
**Prof. Rohit P. John and his team** have published a research article entitled "*A thiosemicarbazone based AIE active fluorescent probe for selective detection of Zn $^{2+}$ and Cu $^{2+}$ in HeLa cells.*" M. Khangwal, A. Bera, **R. P. John**. *Journal of Photochemistry and Photobiology A: Chemistry*, 482, 2027, 117548.

The work demonstrates the use of coumarin thiosemicarbazone based small molecular fluorescent probe for selective detection of $Zn^{2+}$ and $Cu^{2+}$. The detection of $Zn^{2+}$ works by red-shifted fluorescence emission while $Cu^{2+}$ is detected by fluorescence quenching. The detection of $Zn^{2+}$ is achieved as low as $8.57 \times 10^{-7}$ Mand that of the $cu^{2+}$ could be achieved to $6.98 \times 10^{-7}$ M. The probe can also be employed for the detection of both metal ions in HeLa cancer cells up to a concentration of 5 μM.




**Prof. Soumitra Maity and Apurba** have published an article entitled "*Visible Light-Mediated Dearomative Remote Functionalization of Arenes via a Tandem Strain-Release Spirocyclization Relay*". A Samanta, **S. Maity**. *Organic Letters,* 2026 28 (39): 12419–12424.

Tandem strain-release addition cyclization reactions in bicyclo[1.1.0]butanes (BCBs) present a versatile platform for rapidly creating molecular complexity. While lactams and indolinones have been accessed using alkenes and arenes as appendages via this strategy, the dearomative functionalization of arenes remains unexplored. This work demonstrates a photocatalyst-free, visible light-mediated blueprint for the remote functionalization of arenes in tandem with a strain-release framework. Nitrosamines are utilized as versatile reagents for installing sulfonamides and oximes, leading to intricately designed 3D spirocyclic structures bearing medicinally relevant functionalities.

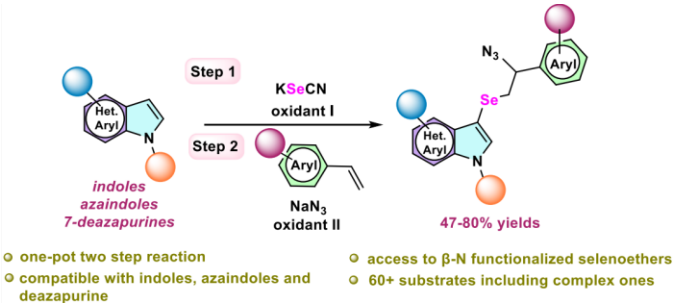



A review article published from the same group titled "*Bicyclo[1.1.0]butane: A Flexible Template for Strain-release Functionalization in Cyclobutane Synthesis*" A. Mukherjee, **S. Maity**. *Synthesis,* 2026; 58(19): 2195-2231.

Bicyclo[1.1.0]butanes (BCBs) are versatile strain-release substrates that enable the conversion of strained σ-bonds into functionalized cyclobutanes. Their high ring strain allows diverse transformations with excellent regio-, diastereo-, and enantioselectivity, broad functional-group tolerance, and mild conditions. This review highlights recent advances in BCB functionalization through Lewis acid, metal-catalyzed, photocatalytic, dual photo/metal, and electrocatalytic strategies, focusing on reaction design, mechanisms, and substrate scope. These developments establish BCBs as valuable building blocks for accessing complex, three-dimensional molecular architectures.



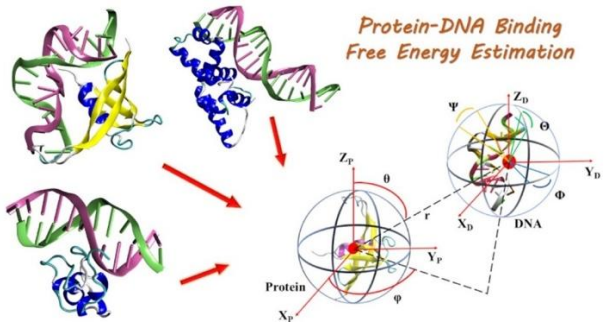
**Prof. Somnath Yadav and his team** have published a research article *"Regioselective β-Azidoselenoalkylation of Indoles, Azaindoles, and 7-Deazapurines via a Two-Step, One-Pot Protocol."* Herein, we report the synthesis of β-azidoselenoalkylation of indoles, azaindoles, and deazapurines via a one-pot reaction involving two sequential steps regioselective addition of the selenocyanate to heterocycles such as indole, azaindole, and 7-deazapurine using KSeCN, followed by the incorporation of the azidoalkyl group from styrenes and sodium azide. The two steps are mediated by two different oxidants, which have been optimized. R. Bera, A. Bhattacharya, R. Paramesh, **S. Yadav**. *Journal of Organic Chemistry,* 91, 11931, 2026.




**Prof. Madhulika Gupta and Ankit Joshi** have published a research article *"Impact of substitution pattern, surface polarity, and temperature in modulating xylan-cellulose interactions."* A. Joshi and **M. Gupta**. *Cellulose*, 33, 5721-5741, 2026.

A review article published from the same group entitled *"Enhancing cellulose extraction efficiency from lignocellulosic biomass: a review of current techniques and microstructural dynamics."* R. Singh, A. Joshi, T. Kundu, **M. Gupta** and M. Patel. *Cellulose*, 33, 5009-5074, 2026.

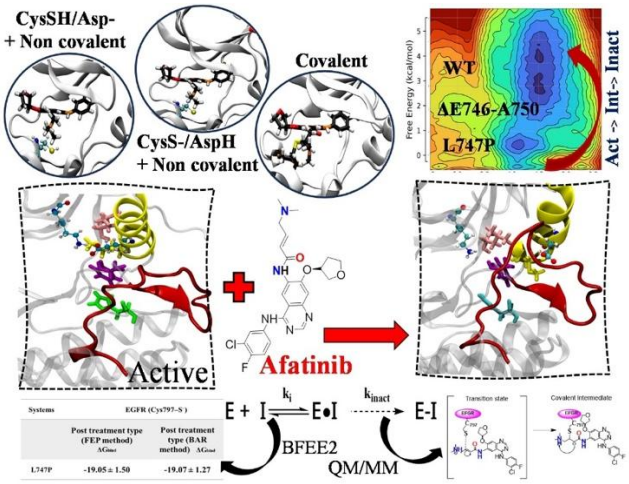
**Prof. Niladri Patra and his team** published a research article entitled "*Estimation of Absolute Protein-DNA Binding Free Energy using Streamlined Geometric Formalism."* Shreya Mukherjee, Diship Srivastava, and **Niladri Patra**. *J. Phys. Chem. Lett.* (2026) 17 (29), 8458–8462.
Protein–DNA complexes play essential roles in gene regulation, replication, transcription, packaging, rearrangement, and DNA repair. Here, we developed a streamlined geometric formalism for accurately computing the absolute binding free energy of protein–DNA complexes. The approach employs a series of potential of mean force simulations using the hybrid Gaussian-Accelerated Well-Tempered Metadynamics-Extended Adaptive Biasing Force (GaWTM-eABF) method, with harmonic restraints on the positional and orientational degrees of freedom of the bound complexes to reduce configurational entropy and overcome sampling limitations. The formalism was applied to three protein–DNA complexes and provided accurate absolute binding free energies at modest computational cost. Interaction analysis revealed that hydrogen bonding, electrostatic, van der Waals, π-cation, and hydrophobic interactions contribute substantially to complex formation. Overall, this geometric framework provides an efficient and accurate computational strategy for estimating absolute protein–DNA binding free energies.




Another research article entitled "Mutation-Dependent Conformational Dynamics and Dual-Mode Afatinib Binding in EGFR Exon 19 Variants." published from the same group. Kousik K. Bhanja, Rajesh Ghosh and **Niladri Patra.** *J. Phys. Chem. B* (2026) 130 (38), 9776–9791.

EGFR exon 19 mutations, particularly ΔE746-A750 and L747P, are clinically important drivers of non-small cell lung cancer. We investigated their effects on kinase conformational dynamics, afatinib binding, and Cys797-mediated covalent inhibition using molecular simulations, alchemical free-energy calculations, and QM/MM methods. Both

mutations favored active-like EGFR conformations but through distinct mechanisms: ΔE746-A750 increased P-loop and ATP-pocket heterogeneity, whereas L747P restricted αC-helix and activation-loop dynamics and more strongly stabilized the active-like state. Afatinib altered the K745-E762 interaction and αC-helix conformation, while the covalent state promoted αC-out configurations and enhanced accessibility of an adjacent pocket. Mutation- and protonation-dependent differences in afatinib binding free energies and Cys797 reaction barriers were observed, with L747P exhibiting a lower calculated barrier than ΔE746-A750. These findings demonstrate that distinct exon 19 mutations reshape EGFR conformational landscapes and the energetic environment of covalent inhibition, providing a mechanistic basis for mutation-dependent afatinib responses.




**Prof. Parthasarathi Das and his group** published a research article entitled "*Introducing Azaindole Thianthrenium Salt: An Electrophilic Coupling Partner for Cross-Coupling Reaction.*" Siddhartha Paul, Vishal Talukdar, and **Parthasarathi Das**. *Organic Letters,* 2026, 28, 11205−11210.

Another research article published from the same group entitled "*Late-Stage Hydroxycarbonylation of Aryl Thianthrenium Salts Utilizing Chloroform-COware Chemistry.*" Arijit Jash, Ashif Iqubal, and **Parthasarathi Das**. *Journal of Organic Chemistry, 2026, 91, 9328−9340.*

**Prof. Biswajit Chowdhury and his team** published a research article entitled *"Highly Efficient Zr/SBA-15 Catalyst for Solvent-Free Synthesis of Cyclic Carbonates from $CO_2$ and Epoxides at Atmospheric Pressure."* Nitesh Kumar, Akash Mandal, Sumanta Mondal, Asim Bhaumik, **Biswajit Chowdhury**. *New J. Chem.* 50, 12098–121172026.

# Publication list

- Nitesh Kumar, Akash Mandal, Sumanta Mondal, Asim Bhaumik, **Biswajit Chowdhury**. *New J. Chem.* 50, 12098–12117, 2026.
- M. Khangwal, A. Bera, **R. P. John.** *Journal of Photochemistry and Photobiology A: Chemistry*, 482, 117548, 2027.
- Siddhartha Paul, Vishal Talukdar, and **Parthasarathi Das**. *Org. Lett.* 28, 11205−11210, 2026.
- Arijit Jash, Ashif Iqubal, and **Parthasarathi Das.** *J. Org. Chem.* 91, 9328−9340, 2026.
- R. Bera, A. Bhattacharya, R. Paramesh, **S. Yadav.** *J. Org. Chem.* 91, 11931, 2026.
- A Samanta, **S. Maity.** *Org. Lett.* 28 (39), 12419–12424, 2026.
- Mukherjee, **S. Maity.** *Synthesis* 58(19), 2195-2231, 2026.
- Joshi and **M. Gupta.** *Cellulose*, 33, 5721-5741, 2026.
- R. Singh, A. Joshi, T. Kundu, **M. Gupta** and M. Patel. *Cellulose*, 33, 5009-5074, 2026.
- Shreya Mukherjee, Diship Srivastava, and **Niladri Patra**. *J. Phys. Chem. Lett.* 17 (29), 8458–8462, 2026.
- Kousik K. Bhanja, Rajesh Ghosh and **Niladri Patra.** *J. Phys. Chem. B* 130 (38), 9776–9791, 2026.

# Workshop Organized

**Gurudakshta (Faculty Induction Programme): Prof. Rohit P. John, Dept. of Chemistry and Chemical Biology** and Prof. R. Thangavel, Dept. of Physics as co-coordinators organized an outreach workshop, Gurudakshta (Faculty Induction Programme, No. OCEP 0104 O) from 3rd July to 29th July 2026 (24 days), intended for freshly recruited faculties of higher education institutions. The programme was attended by 46 newly joined faculties from 20 HEIs across the country. The workshop was fully online and had 96 interactive lectures from 50 eminent academicians as resource persons, from reputed institutions. The various topics covered under 10 modules were

Module 1: Higher Education and its Ecosystem

Module 2: Curriculum designing, Outcome based learning and Choice based credit system

Module 3: Teaching, Learning and Assessment

Module 4: Technology for Teaching and assessment of I-generation

Module 5: Personal-Emotional Development and Counselling

Module 6: Research, Professional Development and Academic Leadership

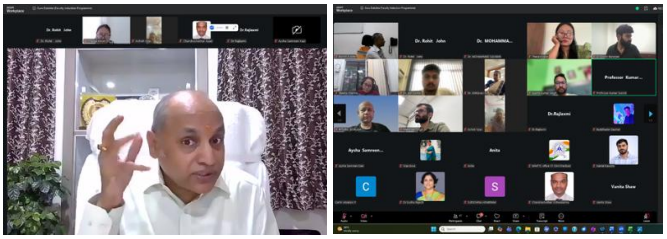
Module 7: Academic Integrity

Module 8: Constitutional Values, Human Rights & Fundamental Duties

Module 9: Environmental Consciousness and Sustainable Development Goals

Module 10: Strategic Planning and Management

The workshop provided a platform for the young faculties an opportunity to recognize and understand the challenges in the higher education sector and made aware of the pedagogical and leadership skills they need to cultivate, and among students so as to equip them for the future.



Prof. Asheesh Srivastava, Dept. of Educational studies, University of Lucknow and faculty participants

**Workshop on *Coagulation and Flocculation of Coal and Iron Ore Fines*:** A half-day Workshop organized at ***Tata Steel Limited, Jamshedpur*** by **Prof. Sagar Pal** on 30th September 2026.

A half-day workshop on "*Coagulation and Flocculation of Coal and Iron Ore Fines*" was organized by Prof. Sagar Pal, Department of Chemistry and Chemical Biology, IIT(ISM) Dhanbad, at Tata Steel on 30th September 2026. The workshop focused on the fundamentals and mechanisms of coagulation and polymeric flocculation, highlighting the role of polymeric reagents in mineral beneficiation, particularly in the processing of fine coal and iron ore particles. The discussions covered mineral surface properties, polymer–mineral interactions, flocculation mechanisms, and the influence of reagent characteristics and water chemistry on process performance. Emphasis was also given on the practical aspects of reagent selection and optimization, with key performance parameters such as settling rate, overflow clarity, underflow density, solid–liquid separation, and dewatering efficiency. The workshop highlighted the potential of polymer-based approaches to improve beneficiation efficiency, enhance water recovery, and support more sustainable mineral processing operations.

**DICE Programme: Mentoring PM SHRI Schools** **Prof. Madhulika Gupta** as PI and Prof. Ejaz Ahmad as co-PI conducted ten sessions across five PM SHRI Schools (UPG HS Dumaria, Mahendra HS Barwa East, UPG HS Dangepara, Govt 2 HS Dhanbad and UPG HS Birajpur) during 16-30th September 2026 under the Ministry of Education's Developing Innovation Culture and Entrepreneurship (DICE) programme. The

sessions covered Developing Entrepreneurial Skills by visiting different schools and Field Visit to i2h for Idea Creation. These activities encouraged creative thinking and entrepreneurial skills among school students. The programme also includes prototype and business model development, awareness of start-up support and intellectual property rights, and a district-level prototype exhibition.







PM SHRI school students visiting i2h under DICE Activity 2: Field Visit and Idea Creation.

**Vigyan Jyoti Programme: Empowering Girls in STEM**

**Prof. Madhulika Gupta**, Nodal Officer, Vigyan Jyoti program under the Department of Science and Technology's Vigyan Jyoti initiative organized visit of 191 girl students from Jawahar Navodaya Vidyalaya (JNV), Koderma, and JNV Dhanbad on 12th August 2026. Another visit of 120 girl students from JNV Burdwan and JNV Jamtara was organized on 2nd September 2026**.** participated. The programmes featured welcome address by Prof. MK Singh (Dean, Faculty) and Prof. Parthasarathi Das (Dean, R & D) and expert talks by Prof. Alok Das (Dean, ICR), Prof. Sanjiv Sahu (AD, SWB), Prof. Sunil Pulletikurthi (CCB), Prof. SR Samadder (ESE), Prof. Scindhiya Laxmi (M n C), Prof. Suresh P. Elumalai to inspire students to explore research and career opportunities in Science, Technology, Engineering and Mathematics (STEM).



Vigyan Jyoti Programme: 12 August 2026




Vigyan Jyoti programme:02nd September 2026

**Swachhata Hi Seva 2026 (SHS2026): Campus Cleanliness Drive**

**Prof. Madhulika Gupta** as Nodal coordinator of SHS2026 along with Center of Societal Mission, EIACP and other faculty members, staff, students and sanitation workers has been engaged in promoting campus cleanliness and public places for a cleaner India.

**Smart India Hackathon (SIH2026):**

The Institution's Innovation Council (IIC), in collaboration with NVCTI, organized a 12-hour internal hackathon for Smart India Hackathon (SIH) 2026 at IIT (ISM) Dhanbad, witnessing enthusiastic participation from 714 students across 119 teams. Students developed innovative solutions to 85 real-world problem statements spanning diverse technological and societal challenges. Following evaluation by a 24-member jury including Prof. Sourav Dey and Prof. Sunil Pulletikurti from CCB , 50 teams were selected for the national round, with the event coordinated by Prof. Madhulika Gupta (Convenor), Prof. Haswant Wundavilli (Co-Convenor), Prof. Omkar Maypati (Coordinator), Prof. Arun Dayal Uday and the NVCTI team under the leadership of Prof. Alok Das (Dean, ICR).

# Research Talks

**Prof. Sagar Pal** delivered an invited talk on "*Functional Polymers: Designing Materials for Industrial Applications*", CRVSB – 2026, Salt Lake Guest House, IISER Kolkata, 03-04 July 2026.

**Prof. Soumitra Maity** delivered an invited lecture on the topic: *"Harnessing Chemodivergency through Photocatalysis"* held on 17th August in the National Symposium on Organic Chemistry-V (NSOC-V) at Jadavpur University.



**Prof. Soumitra Maity** delivered an invited lecture on the topic: *"Manipulating Reactivity Paradigms by Photocatalysis"* held on 19th August in the ICOS Session at the XXV NOST-OCC at Goa.




**Prof. Soumitra Maity** delivered an invited lecture on the topic: *"Multifaceted Photocatalytic Strategies for 3D-Molecular Scaffolds"* held on 24th September in the International Conference on Organometallics and Catalysis (ICOC-IV 2026) in Goa.




**Prof. Madhulika Gupta** delivered lecture on "Education and Research: Impact of Outreach Programs" at the GuruDakshta Faculty Induction Programme, organised under the Malaviya Mission Teacher Training Centre at IIT (ISM) Dhanbad, on 26th July 2026.

**Prof. Niladri Patra** delivered an invited talk on "*pH-Responsive Dynamics Govern OprM Pore Opening in the MexAB-OprM Efflux Pump: Biophysical Insights into Drug Expulsion Modulation*" in One-day International Science Conference and Students' Scientific Competition at Ramakrishna Mission Vivekananda Centenary College on 20 August 2026.

**Prof. Santosh Gharpure, IIT Bombay** delivered an invited talk on "*Advancing MHAT Radical Chemistry for Carbo- and Heterocycle Synthesis*" at the APC Roy seminar Hall, Dept. of Chemistry and Chemical Biology on 18th September 2026.



# Awards & Recognitions

**Prof. Naga Rajiv Lakkaniga** is appointed as Scientific Advisor- R&D at SiBiolead LLC

**Prof. Madhulika Gupta** was selected for the prestigious Schmidt AI in Science Faculty Fellowship at the University of Oxford, 2026. She is one of only three scientists from India and the only woman selected for this highly competitive fellowship.

**Prof. Soumitra Maity and Partha Pratim Mondal**. A patent was granted (Patent #603073) entitled "A novel bifunctional Formyl-amination equivalent reagent, a process for the preparation thereof, and

the application thereof in the synthesis of 1,2-iminoacetals/ß-amino aldehydes"



4 Regional

The Guardian Chronicle, Ranchi, Wednesday, Oct

**IIT (ISM) Dhanbad researchers get patent for new chemical synthesis method**

New technique uses visible light to produce useful chemical compounds under mild conditions, with potential applications in medicinal research

आईआईटी आईएसएम के शोधकर्ताओं को नई रासायनिक विधि के लिए मिला पेटेंट

क्या है नई तकनीक

**Prof. Madhulika Gupta** and her team published a patent entitled "A Green Deep Eutectic Solvent-Mediated GO-$Fe_3O_4$ Heterostructure Derived from Low-Grade Indian Coal for Degradation of Pharmaceutical Pollutants". Sarita Yadav, Suprabha Palatasingh, **Madhulika Gupta**, Shariq Farhan Elahi, Ejaz Ahmad, Afaq Ahmad Khan. Indian Patent Application No. 202631102108, 4th September 2026 (Published).

## Research Grant details

**Prof. Niladri Patra** received funding of INR 1.4 Cr on "Predictive Tools for Antibiotic Discovery in Klebsiella pneumoniae" from the Gates Foundation, Seattle, USA.

Ministry of Education's awarded IIT(ISM) Dhanbad with a grant of Rs. 6,20,000/- with **Prof. Madhulika Gupta** as PI and Prof. Ejaz Ahmad as co-PI for Developing *Innovation Culture and Entrepreneurship (DICE)* programme for mentoring *five PM SHRI Schools*.

**Prof. Madhulika Gupta** received a grant of ₹19,47,316/- from TEXMiN for the project "AI-Empowered Multiscale Framework for Sustainable Rare-Earth Recovery from Secondary Sources", for May 2026–October 2027, as Sole Principal Investigator.

## Centenary Early Career Faculty

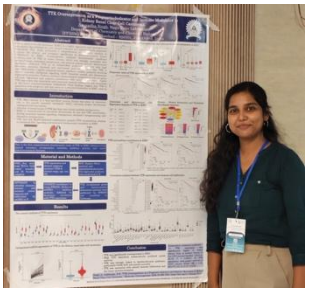
**Dr. Aisha Noor, Dr. Rupak Chatterjee** and **Dr. Shuvojit Mandal** joined as a *Centenary Early Career Faculty* in the Department of Chemistry and Chemical Biology.

# Student Spotlight



**Apurba Samanta,** Ph.D. student of Prof. S. Maity has successfully defended his thesis entitled *"Visible Light-Induced Photochemical C-N Bond Formation"* on 18th September 2026.

**Ms. Neelanjana Ghosh,** Ph.D. student of Prof. Biswajit Chowdhury has been selected for prestigious CII-ANRF Prime Minister's Fellowship for Doctoral Research.



**Anuradha Singh**, PhD student in Prof. Lakkaniga's lab, won the best poster presentation at BIOSPAN-2026 conference at IIT Bhilai.




**Arup Bairagi**, Ph.D. student of Prof. S. Yadav presented a poster at the prestigious Belgian Organic Synthesis Symposium (BOSS XIX) held between July 5th–10th, 2026 at KU Leuven, Belgium.

**Tripti Kundu**, Ph.D. student of Prof. M. Gupta was awarded the PhD degree on 24 August 2026.

**Ms. Shreya Mukherjee,** PhD Student of Prof. Niladri Patra, attended ACS150 Symposium on 1st July, 2026 IACS, Kolkata.

**Dr. Madan Kumar** (Ph D IIT Ropar) joined the Department as ANRF-National Post Doctoral Fellowship (N-PDF) under mentorship of Prof. Parthasarathi Das.

# Editorial Board



**Chief editor:** Prof. Sagar Pal (HOD)





**Editor:** Prof. Sunil Pulletikurti (Assistant Professor); Prof. Ananya Banik (Assistant Professor)

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***Website:***

https://www.iitism.ac.in/department-of-chemistry-and-chemical-biology

***Contact:***

0326-223-5281

***Email:***

*officeofccb@iitism.ac.in*