

From the HOD's Desk

Greetings !

It is with great pleasure that I welcome you once again and present the latest edition of our departmental newsletter, "*Chemistry Connect*". On behalf of the faculty, staff, and student community of the Department of Chemistry and Chemical Biology, I am proud to continue sharing our journey of academic excellence, innovative research, and collective accomplishments. In our previous edition, we celebrated a host of exciting developments—from the vibrant launch of charming Chemistry Buzz, to the remarkable achievements of our students, and successful collaborations across various domains. This edition offers yet another inspiring glimpse into our recent strides and milestones. Inside, you'll find notable achievements, and meaningful contributions that reflect the passion, dedication, and perseverance of our community. I encourage you to immerse yourself in the vibrant academic and research culture that defines our department.

Here is my heartfelt thanks to our committed faculty and enthusiastic students, your tireless efforts continue to drive our department forward. As always, we welcome your valuable suggestions and feedback as we work together to strengthen our shared vision.

Warm regards,

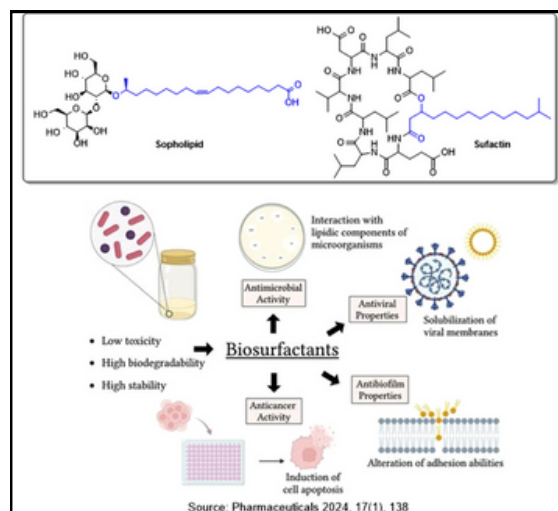
Prof. Parthasarathi Das

Head of Department



Chemistry Buzz

Biosurfactants are amphiphilic molecules and secondary metabolites produced by microorganisms such as bacteria, yeast, and fungi. Because of bioavailability, self-assemble behaviour at lower critical micellar concentrations (CMCs) and low toxic nature, biosurfactants have been widely used as drug carriers in medicinal industry and in other applications such as cosmetics, food and oil industries. Sophorolipid and Surfactin are among with various types of biosurfactants have been widely studied toward antitumor activity. Sophorolipid (a type of glycolipid) was shown to induce apoptosis in H7402 Human liver cancer cells by activating caspase-3 and increasing Ca^{2+} concentration in the cytoplasm. Surfactin (a type of lipopeptide) blocks cell proliferation (by inducing proapoptotic activity) and the PI3K/Akt signalling pathway. Chemical derivatisation of sophorolipid and surfactin were also shown to have anticancer activities.



Spotlight



Dr. Sunil Pullettikurti

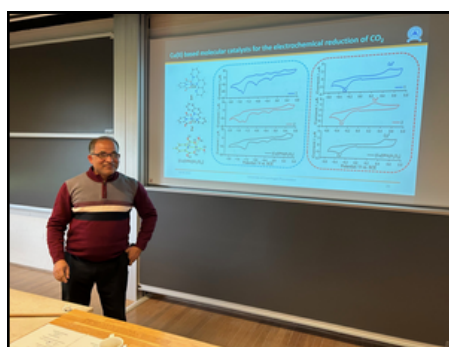
Dr. Sunil Pullettikurti joined the department as an Assistant Professor in April 2025. He earned his M.Sc. in Organic Chemistry from Andhra University (2012) and completed his Ph.D. in organic synthesis and methodology at IIT Bombay (2020) under Prof. Sambasivarao Kotha. He then pursued postdoctoral research at the Scripps Research Institute, USA (2020–2025) with Prof. Ramanarayanan Krishnamurthy, focusing on chemical origins of life and the transition of small biomolecules into life-like systems under early Earth conditions. In 2023, he received a NASA postdoctoral fellowship to explore metabolic pathways in model protometabolic cell compartments. His work has been featured in multiple science news outlets. His current interests include designing novel phospholipids for drug delivery and biological compartmentalization.

Publications

1. Tiwari, M. K.; Muskan and Das, P.*, Pd(II)-Catalyzed Tandem Intramolecular Oxidative Heck Reaction/ C–H Arylation Sequence: One-Pot Synthesis of 3-Nitro-2-Aryl-Indoles. *Asian. J. Org. Chem.*, **2025**, *14*, 5, e202400692; DOI: 10.1002/ajoc.202400692.
2. Talukdar, V.; Paul, S.; Mondal, K. and Das, P.*, CuF₂-Catalyzed C–N Cross-Coupling of Aryl Silanes: Expanding the Scope of Chan-Lam Type Reaction. *Adv. Syn. Cat.*, **2025**, *367*, e202401498; DOI: 10.1002/adsc.202401498.
3. Roy, T.; Mondal, K.; Halder, P.; Sengupta, A. and Das, P.*, CuF₂/DTBP-Catalyzed Chan-Lam Coupling of Oxazolidinones with Arylboronic Acid Pinacol Ester: Scope and Application. *J. Org. Chem.*, **2025**, *90*, 18, 6219–6232; DOI: 10.1021/acs.joc.5c00283.
4. Patra, S.; Samanta, S.; Talukdar, V. and Das, P.*, HFIP-Promoted Regioselective Hydrofunctionalization of Enamides and N-Vinyl Azoles. *J. Org. Chem.*, **2025**, *90*, 18, 6261–6277; DOI : 10.1021/acs.joc.5c00378.
5. Kumar, M.; Chakraborty, S. and Nayek, H. P.*, Organotin(IV) Compounds Catalyzed Cyanide-free Synthesis of α -Iminonitriles. *Dalton Trans.*, **2025**, *54*, 8470-8482; DOI: 10.1039/D5DT00492F.
6. Ahmad, I.; Zamindar, S.; Banerjee, P. and Yadav, M.*, Detailed experimental and quantum chemical investigation on polysaccharide derived from Gellan Gum as a potent and green corrosion inhibitor for mild steel in 15 % HCl. *International Journal of Biological Macromolecules*, **2025**, *317*, 144607; DOI: 10.1016/j.ijbiomac.2025.144607.
7. Mutahir, K. M.; Kumar, S.; Sarkar, T. K.; Saraswat, V.; Obot, I. B.* and Yadav, M.*, Gravimetric, electrochemical, and theoretical investigation of thiourea-based corrosion inhibitors for mild steel in 15% HCl at low concentrations. *Journal of Industrial and Engineering Chemistry*, **2025**; DOI: 10.1016/j.jiec.2025.05.007.
8. Dorandish, S.; Bhayekar, K.; Singh, A.; Kushwaha, N. D.; Malin, E.; Serafimovski, S.; Kelm, J. M.; Gavande, N. S. and Lakkaniga, N. R.*, Evolution of structure-guided drug design strategies targeting mutations in codon 12 of KRAS. *RSC Medicinal Chemistry*, **2025**; DOI: 10.1039/D5MD00169B.
9. Chakraborty, G.; Kolpe, M. S.; Nath, I. V. A.; Tiwari, A.; Jayaswal, P. and Patra, N.*, Computational structure-guided approach to simulate delamanid and pretomanid binding to mycobacterial F420 redox cycling proteins: identification of key determinants of resistance. *Journal of Biomolecular Structure and Dynamics*, **2025**; DOI: 10.1080/07391102.2025.2498621.
10. Paul, D.; Sahoo, P.; Pradhan, A. K.; Datta, P. K.; Sengupta, A.; Tripathy, U. and Chatterjee, S.*, Revealing the importance of the C(1) position to modulate the photophysics and Z-scan responses of o-locked GFP chromophores. *J. Chem. Phys.*, **2025**, *162*, 23, 234308; DOI: 10.1063/5.0274692.
11. Mishra, A.; Makhal, K.; Raj, D.; Pasupalak, S.; Mallik, B. S.*; Nordlander, E.* and Padhi, S. K.*, Hydrogenation of CO₂ to Methanol by a Nickel Pincer Catalyst and Mechanistic Investigations by DFT Studies. *Eur. J. Inorg. Chem.*, **2025**, e202500138; DOI: 10.1002/ejic.202500138.

Invited Lectures

1. On 2nd June 2025, Dr. S. K. Padhi delivered an invited lecture at the Department of Chemistry, University of Copenhagen, Denmark, titled "Understanding Cu(II)-Driven CO₂ Electroreduction: Competition and Synergy with Proton Reduction." The presentation focused on elucidating the mechanistic pathways governing Cu(II)-mediated electrochemical CO₂ reduction and its interplay with concurrent proton reduction processes. The talk was well-received and followed by a productive discussion with Professor Dr. Jiwoong and Professor Craig S. Day, leading to promising dialogues on prospective research collaborations in the field of electrocatalysis and energy conversion.



Dr. S. K. Padhi delivering invited talk at the University of Copenhagen, Denmark



Dr. S. K. Padhi with Professor Dr. Jiwoong and Professor Craig S. Day

2. Dr. S.K. Padhi delivered an invited research talk at the Department of Chemistry, Lund University, Sweden, on 12th June 2025, on the title "Proton vs. CO₂: Understanding the Selectivity Switch between Cu(II)- and Co(II)-Catalyzed Electroreduction." The lecture addressed the mechanistic factors governing product selectivity in metal-catalyzed electrochemical reduction processes, with a particular focus on the divergent pathways facilitated by Cu(II) and Co(II) complexes. The session concluded with a highly engaging discussion, including fruitful scientific exchanges with Professor Isaac Garcia-Bosch (Carnegie Mellon University, USA) and Professor Petter Persson (Lund University), opening avenues for future collaborative research in molecular electrocatalysis and reaction mechanism design.



Dr. S.K. Padhi delivering invited talk at LUND University, Sweden



Dr. S. K. Padhi with Prof. Ebbe Nordlander and Professor Isaac Garcia-Bosch (Carnegie Mellon University, USA)

Events Organized

A one-day seminar on “**Chemical and Biochemical Industry Meet 2025**” was organized on the 3rd May, 2025, in the Department of Chemistry and Chemical Biology, IIT (ISM) Dhanbad under the mentorship of Prof. Parthasarathi Das (HOD, CCB) and Prof. Swapan Dey (Coordinator). The significance of this ‘Chemical and Biochemical Industry Meet 2025’ lies in its role as a platform for stakeholders in the chemical and biochemical sectors to exchange knowledge, discuss trends, and address key challenges within these industries. It serves as a key event for driving innovation, shaping policy, fostering partnerships, and advancing the sustainability of the participants.



Director [IIT (ISM) Dhanbad], Professors [CCB, IIT (ISM) Dhanbad] and invited business leaders at “Chemical and Biochemical Industry Meet 2025”

Celebrating the Legacy of Prof. Udayabhanu G.

The Department of Chemistry and Chemical Biology, IIT (ISM) Dhanbad, proudly celebrated the exceptional 37-year journey of **Prof. Udayabhanu G.**, fondly known as **GU Sir**, who served the department with unwavering dedication since 1988. The farewell event was held on 30th May 2025 at GJLT, featuring a scientific session, a felicitation ceremony in his honor. The department came together to express gratitude for his invaluable teaching, research, and mentorship contributions over nearly four decades.



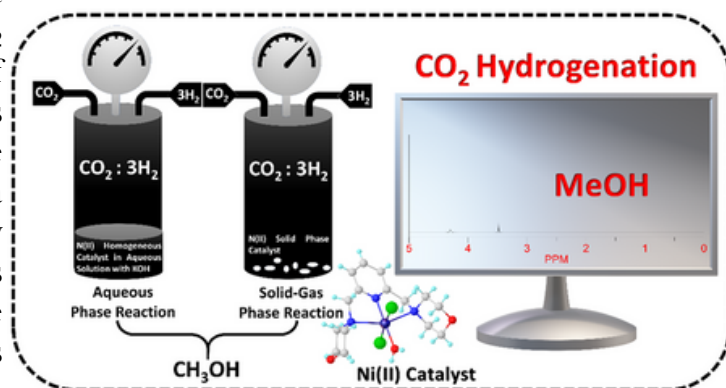
Bidding farewell to 37 years of wisdom and warmth - GU Sir with students and colleagues

Celebrating contribution of Mr. C. Devid

The department gratefully acknowledges the dedicated service of Mr. C. Devid, Scientific Officer, for his over 30 years of valuable contribution.

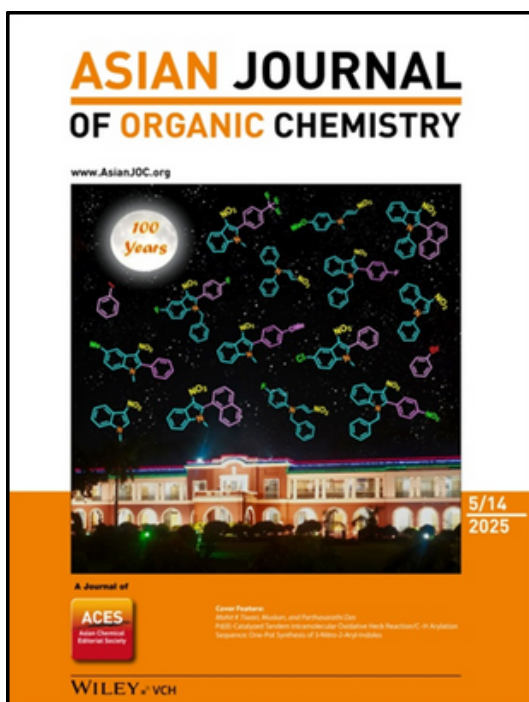
Other Achievements

1. Prof S.K. Padhi's group highlighted their recent publication on Nickel Pincer-Catalyzed CO_2 Hydrogenation to Methanol in *European Journal of Inorganic Chemistry* (2025, e202500138). This article reports a detailed investigation into the hydrogenation of CO_2 to methanol mediated by a nickel pincer complex. The study systematically compares the catalytic performance under aqueous and solid-gas phase conditions at moderate temperatures (60–95 °C). The solid-gas phase was found to be significantly more efficient, yielding up to 18 μmol of methanol at 95 °C and 1 MPa H_2/CO_2 (3:1), compared to 10 μmol under analogous aqueous conditions. The formation of methanol was unambiguously confirmed via $^{13}\text{CO}_2$ labelling in the presence of KOH/KOD . Complementary DFT calculations elucidated the mechanistic landscape of the transformation, supporting the proposed reaction pathway and key intermediates. This study highlights the viability of nickel-based systems for CO_2 hydrogenation and underscores the potential of solid-gas phase catalysis for improving methanol yield under thermodynamically mild conditions.



2. Prof. Parthasarathi Das's work was featured as the Cover Art of the “Asian Journal of Organic Chemistry” (DOI : 10.1002/ajoc.202400692).

3. Prof. Niladri Patra's work was featured on Front Cover of “The Journal of Physical Chemistry B” (DOI : 10.1021/acs.jpcb.4c07651).



Prof. Parthasarathi Das's work was featured as the Cover Art of the “Asian Journal of Organic Chemistry”

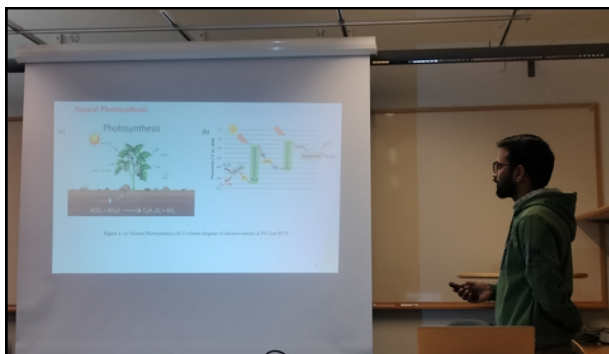


Prof. Niladri Patra's work was featured on Front Cover of “The Journal of Physical Chemistry B”

4. **Prof. Madhulika Gupta** was nominated to attend the Workshop on the Conduct of Inquiry on Complaints relating to Sexual Harassment of Women at the Workplace, scheduled to be held from 5th to 6th May, 2025, at the Institute of Secretariat Training and Management (ISTM), New Delhi.

Students' Achievements

Mr. Dev Raj, PhD student in Dr. S. K. Padhi's Group, delivering a talk at LUND University of Copenhagen, on electrochemical water oxidation by Cu(II) catalysts. He visited LUND university under the bilateral mobility programme in STINT, Sweden, funded project.



Mr. Dev Raj delivering a talk at LUND University of Copenhagen



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Contact: ccb@iitism.ac.in