

CHEMISTRY CONNECT



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Vol 2 Issue 2

From the HOD's Desk

Most welcome!**Pleased to see you again!**

Here I introduce you to the continuation of our department's academic journey through the debut of our new newsletter, '*Chemistry Connect*'



on behalf of the faculty, staff, and students community of the Department of Chemistry. I invite you to immerse yourself in our dynamic research and educational pursuits. Last time in our newsletter, we shared a range of exciting updates, including the latest on charming buzz, students' remarkable achievements, and notable accomplishments across departments. We're back with another update on our department's latest achievements! Let's take a look at the latest newsletter, where we share inspiring insights and enlightening topics from our department.

We welcome your valuable suggestions and feedback as we strive to elevate the Department to new heights. A big shoutout to our dedicated faculty and students for their hard work and commitment throughout this academic journey!

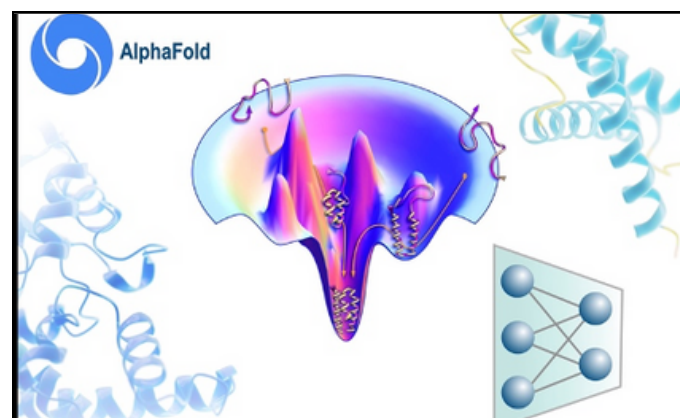
Warm regards,
Prof. Parthasarathi Das
Head of Department

Chemistry Buzz

AlphaFold: Accelerating Breakthroughs in Chemistry with AI

AlphaFold, an AI system developed by Google DeepMind, delivers a groundbreaking achievement in structural biology by solving the long-standing

protein folding problem. For decades, scientists have struggled to predict how a protein's sequence of amino acids would fold into its unique three-dimensional structure, a crucial challenge for understanding biological functions and developing disease treatments. Traditional methods of determining protein structures are time-consuming and expensive. Trained on extensive datasets of known protein structures, AlphaFold leverages advanced machine learning algorithms based on graph neural networks. The latest version of AlphaFold is capable of predicting protein structures solely based on their amino acid sequences with unparalleled accuracy, providing a transformative tool for advancing biomedical research.



Nobel Prize 2024 in Chemistry recognizes the importance of AlphaFold and AI in advancing science. Dr. David Baker from the University of Washington, USA shared the prize with Dr. Demis Hassabis and Dr. John Jumper from Google DeepMind, UK. Dr. Hassabis and Dr. Jumper developed the core architecture of AlphaFold, an algorithm predicting protein's structure from its amino acid sequence. Dr. Baker's contribution lies in his pioneering work on computational design of proteins.

Publications

1. Das, A.; Mandal, S. K.; Kumar, N.; Maity, N.; Kumar, A.; Sinha, S.; Bahadur, J.; Chowdhury, B.*, Sen, D., Diverse Pore Ordering in Porous Silica: Synthesis and Quantitative Structural Insights Combining Scattering and Imaging Techniques. *Phys. Chem. Chem. Phys.* **2025**; DOI:10.1039/D4CP04056B.
2. Mishra, V.K.; Mondal, S. & Haldar, C.*, Synthesis and Characterization of Dioxidovanadium(V) Complexes of Dibasic Tridentate Arylhydrazone Ligands for the Selective Epoxidation of Olefins by Hydrogen Peroxide-Assisted Bicarbonate. *Top Catal.*, **2025**, 1-14; DOI:10.1007/s11244-024-02047-y.
3. Chakraborty, G.; Ojha, K.; Mandal, A.; Patra, N.*, Effect of spacer group variation of gemini surfactants on the detachment of oil from silica surfaces with different hydrophobicity: A molecular dynamics study. *Phys. Chem. Chem. Phys.*, **2025**, 27, 4429-4445; DOI:10.1039/D5CP00248F.
4. Singh, A. and Lakkaniga, N. R.*, Exploring the Conformational Space of MPS1 Kinase Using Metadynamics. *Proteins: Struct. Funct. Bioinf.*, **2025**; DOI: 10.1002/prot.26796.
5. Saraswat, V.; Sarkar, T. K.; Sandhu, N.; Kohli, S.; Rawat, M.; Keshar, K.; Yadav, M.* and Bano, N., Mechanistic Insights into the Corrosion Inhibition Performance of Eco-Friendly Nitrogen and Boron Co-Doped Carbon Dots for Mild Steel in a 15% HCl Solution. *Langmuir*, **2025**, 41, 5, 3528–3540; DOI:10.1021/acs.langmuir.4c04672.
6. Keshar, K.; Mitra, R.K.; Gupta, S.K.; Kumari, P.; Ahmad, I.; Obot, I. B.; Alamri, A. H. and Yadav, M.*, Corrosion inhibition and adsorption behaviour of benzothiazole compounds on mild steel in an acidic environment: Experimental and theoretical approach. *Colloids Surf. A: Physicochem. Eng. Aspects*, **2025**, 136318; DOI:10.1016/j.colsurfa.2025.136318.
7. Maurya, A.; Pradhan, N. and Yadav, M.*, Heteroatom doped MoO₃ as efficient electrocatalyst towards hydrogen evolution reaction in acidic as well as alkaline medium. *J. Electroanal. Chem.*, **2025**, 977, 118827; DOI:10.1016/j.jelechem.2024.118827.
8. Kumar, A.; Kumar, S.; Sarkar, T. K.; Saraswat, V.; Yadav, M.*, Obot, I.B. and Alamri, A.H. Experimental and Theoretical Insights into the Corrosion Mitigation Efficacy of Novel Quinoline-Based Pyrazole and Isoxazole Derivatives. *Colloids Surf. A: Physicochem. Eng. Aspects*, **2025**, 136241; DOI:10.1016/j.colsurfa.2025.136241.
9. Iqbal, A.; Jash, A.; Halder, P. and Das, P.*, Ex Situ Generation of D₂ for Reductive Deuteration: Scope and Application to Late-Stage Functionalization. *J. Org. Chem.*, **2025**, 90, 4, 1571–1584; DOI:10.1021/acs.joc.4c02602.
10. Kundu, T.; Smith, J. C. and Gupta, M.*, Effect of acetylation patterns of xylan on interactions with cellulose. *Biomacromolecules*, **2025**; DOI:10.1021/acs.biomac.4c01469.
11. Roy, A.; Manna, K.; Dey, S.; Chakraborty, K.; Dhara, S. and Pal, S.*, Functionalized amino acid-based injectable hydrogels for sustained drug delivery. *Soft Matter*, **2025**; DOI:10.1039/D4SM01402B.
12. Pradhan, P.; Dey, S.; Manna, K.; Panda, A. B. and Pal, S.*, In situ synthesis of a photocatalyst using TiO₂ QDs-immobilized functionalized galactomannan for degradation of organic pollutant. *J. Water Process Eng.*, **2025**, 69, 106617; DOI:10.1016/j.jwpe.2024.106617.

Sponsored research projects sanctioned

- Title: Preparation of 4-(1H-Pyrrolo[2,3-b]pyridin-4-yl)morpholine (CONS7424C).; Funded by: Tokyo Chemical Industry (TCI), Hyderabad; PI: Prof. Parthasarathi Das.

Invited Lectures

- **Prof. Swapan Dey** and his research group visited to M/S. Alcograin Distillers Pvt. Ltd., Panagrah Industrial Park, West Bengal on the 21st February 2025 as a part of Industry-Academia Interaction.
- **Prof. Niladri Patra** delivered an invited talk on “Methods in Molecular Modelling” in Data Science and Technologies: Applications in Atmospheric and Space Sciences during 20th to 31st January, 2025 at The National Atmospheric Research Laboratory (NARL) – Tirupati.
- **Prof. Sajal Giri** presented an invited poster at the Spectroscopy and Dynamics of Molecules and Clusters (SDMC) conference from 20th to 23rd February 2025, in Mussoorie, India.
- **Prof. Biswajit Chowdhury** was invited to deliver a distinguished talk on “Synthesis of Propene from Propane and Glycerol over Functionalized Catalyst” at the Golden Jubilee Celebration of the Catalysis Society of India (CSI), held from 24th to 26th February 2025 at Thapar Institute of Engineering & Technology, Patiala, Punjab. In addition, Prof. Chowdhury also chaired a technical session, contributing to the discussions on advancements in catalysis research.
- **Prof. Parthasarathi Das** was invited to deliver lectures at the International Conference on Chemistry for Human Development (ICCHD-2025) at Calcutta University, Kolkata (January 4-6, 2025) and the International Conference on Advances in Organic Chemistry (AOC-2025) at IIT Indore/NISER Bhubaneswar, Goa (January 27-29, 2025), showcasing his significant contributions to the field of organic chemistry.



Prof. Biswajit Chowdhury at CSI Golden Jubilee Celebration



Prof. Swapan Dey and his research group



Prof. Sajal Giri at SMDC-2025

Events Organized

- Prof. Biswajit Chowdhury, as the Project Coordinator, organized the kick-off meeting for the institute-level Indo-Norway project titled “Bioscopy – Towards Modern Transdisciplinary Education and Research in Microscopy.” The meeting was held from 13th to 15th January, 2025, in collaboration with the IRAA office.
- Prof. Madhulika Gupta organized the exposure visit to IIT (ISM) Dhanbad for the students of JNV Kalpathar (West Bengal) on 6th February, 2025 and students from JNV Deoghar (Jharkhand) on 10th February, 2025,
- Prof. Madhulika Gupta organized the MR & MISS INDIA 2025 Audition, which took place on February 9th, 2025, at GJLT, IIT (ISM) Dhanbad under the banner of Feel Star.

• SRIJAN & Industry Institute Interaction (III) 2025

Prof. Madhulika Gupta, co-convenor, Srijan 2025 with her students Ankit Joshi, Tripti Kundu, Suprabha Palatasingsh, Reetika Tamang, Vivek Semwal and Uday Bhan organized the inaugural session of SRIJAN 2025. The same team also managed Industry Institute Interaction (III) 2025. Aritra Shyamal, Subarna Das, and Abhishek Yadav also performed in Srijan 2025.

• Saraswati Puja

The Department organized and celebrated Saraswati Puja on February 2nd 2025. On this occasion, Prof. Sukumar Mishra, Director, IIT (ISM) Dhanbad, along with his wife Mrs. Sakuntala Mishra, visited the department. Prof. R.R. Sonde, IIT Delhi - Abu Dhabi along with his wife, and Ms. Dana Blackman, Head of the India Office, International Business Development, India Brazil Chamber of Commerce graced the occasion of Saraswati Puja in the department.



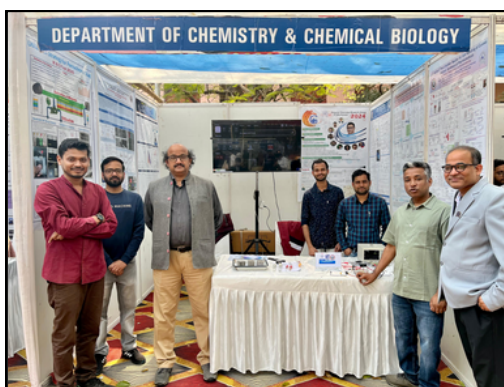
Indo-Norway project meeting



Saraswati Puja 2025



Industry Institute Interaction (III) 2025



Industrial meet 2025



Srijan 2025



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