INTER IISER-NISER CHEMISTRY MEET-2025

IINCM-2025

20-22 March 2025

INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH, PUNE

ABSTRACT BOOK

INSTITUTE OF SCIENCE EDUCATION AND RESEARCH, PUNE

Welcome To IINCM-2025

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T01: Prof. Sunil S. Bhagwat

Affiliation: Director, IISER PUNE

Title: Development of a novel instrument for measuring foamability: TESFAM

Abstract: Foam is a dispersion of gas in liquid which is often undesirable in a process. It can affect measurements, production capacity or product aesthetics. On the other hand, many products use foam to a benefit in terms of volume addition, texture modification, or as a scaffold. Various applications find foam a nuissance and try to avoid it. A distillation or absorption column, pipelines carrying liquids are examples of this kind. Making of styrofoam, insulating foams on the other hand aim at maximising foam and also need foam of a specific type. Additionally, fire-fighting foams and shaving foams also need to be formed within a short duration. The dynamics of micellar break-up, diffusion and adsorption - all can affect the quickness of foam formation.

The accurate measurement of foam properties is quite difficult and is usually divided into foamability - the instantaneous foam formation capability of a solution and foam stability - the long term ability of the foam to remain as such without bubble breakage. The foamability is related to dynamics of surface tension while the stability relates more to viscosity and liquid drainage. Foamability is commonly measured in the industry using Ross-Miles apparatus.

The Ross-Miles apparatus has several shortcomings which will be discussed in this presentation. The main issues are about foam breakage and non-impingement of jet on liquid surface. A new apparatus was developed to overcome these limitations and provide a sensitive and reproducibile measurement of foamability which are required in many applications. The working of this instrument and the reasons for reproducibility and accuracy will be explained. The apparatus involves a continuously wet solid surface and removal of accumulated foam bubbles. Majority of the interfacial area is in fine bubbles and these are segregated from large bubbles. The volume of fine bubbles collected over a period indicates foamability of the test solution. The measurements are reproducible and are able to distinguish between varying concentrations of a surfactant. The effect of various additives is also detected accurately with this apparatus. Thus, the use of foam boosters and antifoaming aents can be tested satisfactorily in this instrument.

Specific applications of these two extremes one where foaming was undesirable and one where high amount of stable foam was needed will be discussed briefly.

Biosketch:

Dr. Sunil S Bhagwat, B.Chem.Engg., M.Chem.Engg., Ph.D.(Tech) is the Director, Indian Insititute of Science Education and Research, Pune since 2023. Earlier, he was a Sr Professor of Chemical Engineering in the Institute of Chemical Technology (earlier known as UDCT/UICT), Mumbai since 1986. There, he held the positions of Dean, Academic Programmes, member, Board of Governors, Coordinator of Centre of Excellence in Process Intensification and PostGraduate Diploma course in Chemical Technology Management. His area of Specialization is Interfacial Science and Engineering, Artificial Neural Networks, Energy and Exergy Engineering. His group has successfully completed several research projects funded by government agencies such as CSIR, DST, public sector bodies such as DAE, NTPC, and by private sector companies such as Hindustan Lever Ltd, MARICO Industries Ltd, ICI, British Petroleum, etc. In 2013, his research group won the first prize in the Bry-Air asia awards for the HVAC for his work in the area of heat based refrigeration. He was awarded NOCIL Award of the Indian Institute of Chemical Engineers for excellence in design or Development of Process Plant or Equipment in 2012 and the CSMCRI-Chemcon Distinguished Speaker Award at Chemcon Dec 2014. He was Elected the best teacher by the students and awarded the Prof. R. A. Rajadhyaksha Best Teacher Award at ICT many times and in 2016, the Indian National Science Academy (INSA) bestowed upon him the best Teacher Award for the year 2016. In 2019, he was selected for the UDCT Alumni Association’s Distinguished Alumnus Award - Academic category. In 2022, he was awarded the K V Mariwala Award for Industry-Academia interactions by the Indian Chemical Council, and in 2023 he was elected the Fellow of the Indian National Academy of Engineering. He is a life member of Indian Institute of Chemical Engineers (past Chairman, Mumbai Regional Center) and the Honourary secretary of the Indian Society for Surface Science and Technology, Western India Chapter. He is also a life member of Oil Technologist’s Association of India. He is on the Editorial Board of the Journal of Surface Science and Technology, India and was on the Editorial Advisory Board of the Industrial & Engineering Chemistry Research of the American Chemical Society between 2013-2015. While at the ICT, he has spent one year at the University of Florida, USA and a semester at Texas Tech University, USA where he contributed to research and teaching. He is a past chairman of the Indian Institute of chemical Engineers (IIChE) Mumbai regional Center and is the Hon Secretary of the Indian Society for Surface Science and Technology, Western India Chapter. He is an active consultant to the chemical industry and the client companies range from pharmaceutical ancillary company to an industrial research company like Tata Research Development and Design Centre to manufacturing companies such as Galaxy Surfactants, MARICO Industries, Balmer-Lawrie, GSK-CH, GAIL, HUL, TRDDC, Thermax, Reliance Industries, IPCA laboratories, UNICHEM laboratories, Jayant Agro-Organics Ltd, KV Fire, DCM-Shriram and PPG Industries, USA. He has presented talks at various university research centers, industries and conferences in India as well as abroad. He has guided 85 masters theses, 45 doctoral theses, has more than 100 international publications and over 80 national/ international conference presentations and 11 national and international patents to his credit.

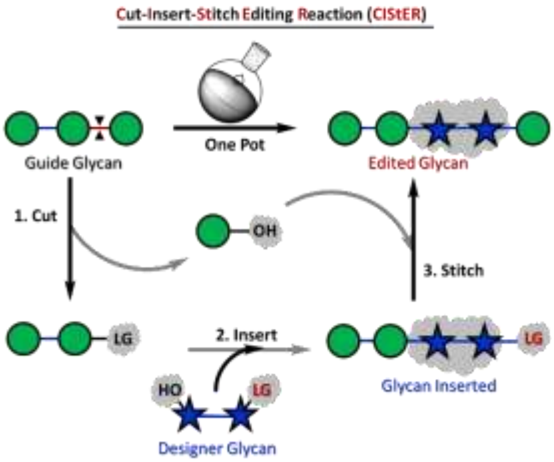
T02: Prof. Srinivas Hotha

Affiliation : IISER PUNE

Title: CIStER: A Chemical Glycan Editing Reaction Sequence

Abstract: Existing strategies for the syntheses of oligosaccharides follow convergent, divergent, chemical or enzymatic routes.[1] Contrary to these, nucleic acids enjoy the unique advantage of PCR, polymerases, and editing methods such as CRISPR[2] which have advanced the field to an unprecedented level. Unlike nucleic acids, oligosaccharides are lagging behind due to inherent challenges in their syntheses.[3]

In this lecture, a working framework will be presented for the editing of oligosaccharides viz. Cut-Insert-Stitch Editing Reaction (**CIStER**) technology that stands on the subtle reactivity patterns (Figure 1).[4]



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Biosketch:

Srinivas Hotha
Professor
Department of Chemistry
Indian Institute of Science Education and Research (IISER), Pune
Contact Number: +91 20 2590 8015
E-Mail: s.hotha@iiserpune.ac.in
Homepage: http://www.iiserpune.ac.in/~s.hotha

Srinivas Hotha earned his MSc (Chemistry) from the University of Hyderabad in 1993, MTech (Biochem Engg) from IT-BHU, Varanasi in 1995 and a Ph. D. in Chemistry from Osmania University in 2001 for the work he carried-out at IICT Hyderabad and NCL Pune. He was a Charles H. Revson postdoctoral fellow at Rockefeller University, New York USA from 2001-03. He returned to India, joined NCL Pune as a scientist and subsequently relocated to Indian Institute of Science Education and Research, Pune in November 2010 wherein he is a Professor since 2016. He co-founded the SciCHEM Innovations Pvt Ltd. in 2024.

His research interests are in the application of sustainable methods for the synthesis of oligosaccharides of biological significance. Notably, he has developed, pioneered and nurtured the gold-catalyzed glycosidation method over the past 20 years.

T03: Prof. Vignesh Kuduva R

Affiliation: IISER MOHALI

Title: Role of 3d/4d-4f magnetic exchange interactions and diamagnetic 3d ions on the magnetic dynamics of Ln(III) ions in heterometallic {3d/4d-4f} Single-Molecule Magnets

Biosketch:

Prof. Kuduva R. Vignesh
Department of Chemical Sciences,
Indian Institute of Science Education and Research Mohali
Email: vigneshkuduvar@iisermohali.ac.in

Kuduva R. Vignesh completed his PhD in 2016 at IITB-Monash Research Academy, IIT Bombay, Mumbai under the joint guidance of Prof. G. Rajaraman (IIT Bombay) and Prof. Keith S. Murray (Monash University, Australia). Later, he worked as a postdoctoral researcher under Prof. Kim Dunbar at Texas A&M University, USA for two years, under Prof. Masahiro Ehara at the Institute for Molecular Science, Japan for one year. After briefly working as a JSPS postdoctoral fellow under Prof. Masahiko Hada at Tokyo Metropolitan University, Japan, he joined as an assistant professor at the Department of Chemical Sciences, Indian Institute of Science Education and Research Mohali in May 2022. His research group at IISER Mohali is focusing on i) low-coordinate Single-Molecule Magnets (SMMs) for higher blocking temperatures to use them as information storage devices and Q-bits, ii) cyclic lanthanide-based Single-Molecule Toroics (SMTs) as quantum spin sensors, and iii) the spin-crossover (SCO) materials for display devices. He designs, synthesizes, and models these molecular magnets using both experimental and computational tools such as X-ray diffractometer, SQUID magnetometer, DFT, and high-level ab initio calculations. Till date he has published 48 papers in high-ranking international journals and two book chapters. He has received “Best Collaborative Student award” from IITB-Monash Research Academy in 2015, and “Excellence in PhD Research Award” from IIT Bombay in 2018, and a SERB-ITS grant in 2024 to attend and present a seminar at ACCC9, Bangkok, Thailand.

T04: Prof. Pushpita Ghosh

Affiliation: IISER TVM

Title: Spatiotemporal dynamics and emergent orders in chemical and biological systems

Biosketch

Dr. Pushpita Ghosh Curriculam Vitae Contact Information

Assistant Professor Grade -1,

School of Chemistry,

IISER Thiruvananthapuram,

Maruthamala P.O., Vithura, 695551, Kerala, India

E-mail: pushpita@iisertvm.ac.in

Office: +914712778308, Mobile: +919160401956

Academic qualification and Professional Experinence:

λ **Assistant Professor**, School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram, India. (September 2021 -) λ **INSPIRE Faculty**, TIFR-Center for Interdisciplinary Science, Hyderabad, India. (August 2016 - August 2021)

λ **Postdoctoral Research Scholar**, University of California Berkeley, USA. (February 2016- August 2016)

λ **Postdoctoral Fellow**, Center for Theoretical Biological Physics, Rice University, USA. (October 2012 - January 2016)

λ **PhD**, Department of Physical Chemistry, Indian Association for the Cultivation of Science, India. (July 2007- August 2012)

λ **B.Sc. (Chemistry)** and **M.Sc. (Specilization in Physical Chemistry),** Department of Chemistry, Visva-Bharati, India. (2005 and 2007)

Academic Honors and Awards:

- ‘International Visiting Faculty Fellowship” by Cluster of Excellence RESOLV EXC-2033 (ID:390677874) funded by the Deutsche

Forschungsgemeinschaft DFG), October 2024.

- Strat-up research Grant by SERB, India, 2022
- Department of Science and Technology-INSPIRE Faculty Award, (2016- 2021).
- Best Poster Prize in the conference, "Theoretical Chemistry Symposium" (December 2010) at IIT Kanpur.
- Qualified GATE-2007 with All India Rank-50.
- Recipient, Junior Research Fellowship (CSIR-JRF) & Senior Research Fellowship (CSIR-SRF) by Council of Scientific and Industrial Research, New Delhi, India (2007 & 2009).
- Recipient Merit Scholarships for B.Sc. and M. Sc. by Visva-Bharati University (2002-2007). (Rank-2)
- Recipient, Merit Scholarships for Class XI & XII by Visva-Bharati University (2001-2002). (Rank-3)
- Recipient, National Merit Scholarship by Government of India in Madhyamik Pariksha 2000. (Rank-46).

Reseach Interest

Self-organized orders or patterns in temporal and spatial domains are ubiquitous in nature. Our research is broadly focused towards investigating and understanding the dynamics of complex systems under far-from equilibrium, leading to a large variety of emerging spatiotemporal orders in the form of spatial patterns, propagating waves, collective motions, phase-separation in physical, chemical and biological systems. How does a system self-organize into a ordered structure under far-from-equilibrium condition? What are the underlying mechanisms and controlling factors which determine the spatiotemporal dynamics? How can external and internal perturbations, feedback govern the spatiotemporal dynamics? In our research we investigate several of these questions aiming towards developing mechanistic and physical understanding using theoretical and computational approaches. We mainly utilize tools of nonlinear dynamics, statistical mechanics, numerical and computer simulations to address various phenomena of self-organization in complex chemical and biophysical systems. Our current interests focused on the following broad areas:

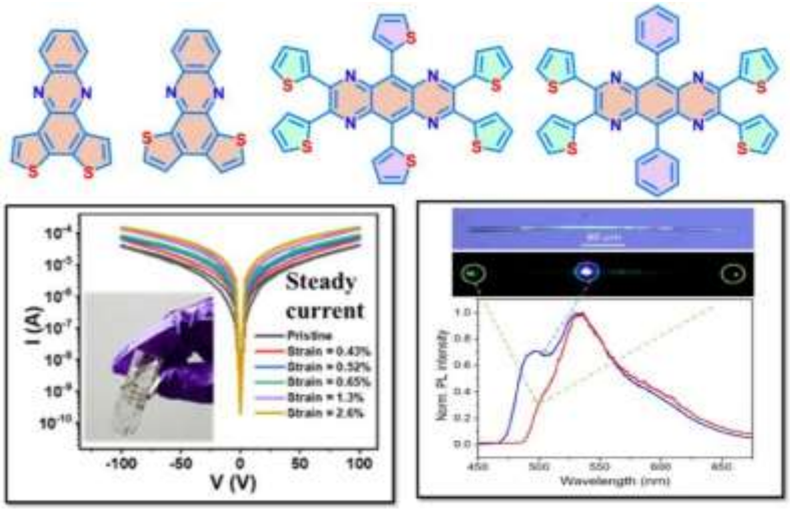
- Nonlinear dynamics of spatially-extended chemical and biological systems: spatiotemporal patterns, oscillations, phase-separation etc.
- Collective dynamics of microbial colonies and multicellular tissues: growth, expansion, migration and self-organization (biomechanics and chemical aspects)
- Non-equilibrium statistical mechanics of active matter and driven systems.

T05: Prof. Sanjio S. Zade

Affiliation: IISER KOLKATA

Title: Thiophene containing phenazine and pyrazinoquinoxaline as organic semiconductors

Abstract: π-Conjugated systems that include conjugated small molecules and polymers have been an integral part of organic electronic devices such as organic photovoltaics (OPVs), organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and organic thermoelectric (OTE). The main prerequisites for using organic semiconductors in printed, flexible electronic devices are (i) high chemical and thermal stability, (ii) high charge-carrier mobility, (iii) solution processability, and (iv) simple synthetic pathways. In addition to molecular design and synthesis, understanding molecular orbital engineering and crystal engineering are crucial for creating the next-generation organic semiconductor. In this context, thiophene-containing phenazine and pyrazinoquinoxaline fused conjugated systems are fascinating candidates. In this talk, synthetic approaches to these intriguing thiophene- containing conjugated systems, their structure-property connection, and their response in organic electronic and photonic devices will be discussed.



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Biosketch:

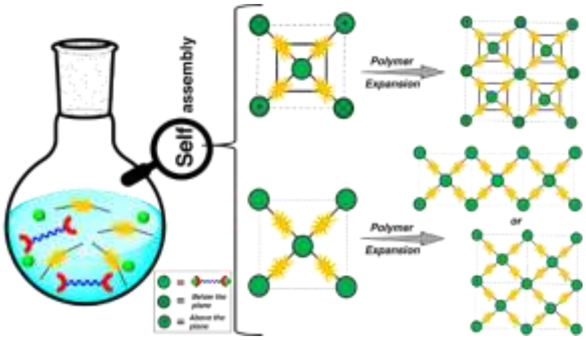
Sanjio S. Zade received his M.Sc. in chemistry from Amravati University in 1997. He received his Ph.D. from the Indian Institute of Technology Bombay (IIT Bombay, 1999-2004), under the supervision of Prof. H. B. Singh. He spent his postdoctoral period in the research group of Prof. Michael Bendikov at the Weizmann Institute of Science, Israel (Feinberg fellowship) (2004-2006). He then joined as a lecturer at the M. S. University, Baroda, in 2006. Subsequently, he moved to Indian Institute of Science Education and Research (IISER) Kolkata in 2007 and currently he is Professor. He is a fellow of Maharashtra Academy of Sciences (FMASc). His research interests include the development of new π-conjugated systems and their applications as materials for energy harvesting and organic electronics.

T06: Prof. Sanjay Mandal

Affiliation: IISER MOHALI

Title: The Room-temperature Self-assembly of Tunable Metal-organic Frameworks Composed of Flexible Neutral Linkers with Six N-donor Atoms and Various Dicarboxylates

Abstract: Understanding and predicting the pathways involved in the synthetic process of metal-organic frameworks (MOFs) comprised of flexible counterparts has always been a challenging task. The complexity increases manifold when a three-component reaction is involved instead of the conventional two-component system. Among the flexible linkers, examples with two, four, and six N-donor atoms have been systematically studied for the effect of denticity and flexibility on the structural features and dimensionalities of the architectures. While the examples of linkers with two N-donor atoms have been reported by many researchers including us, the linkers with six N-donor atoms have been utilized exclusively by our group. In this talk, I will shed light on the self-assembly process of MOFs from a three-component reaction at room temperature involving (a) flexible spanning bis(tridentate) linkers with six N-donor atoms, (b) various linear and bent dicarboxylates, and (c) divalent metal centers for generating 2D or 3D MOFs. In doing so, I will establish the factors - flexibility and angularity of dual linkers - that govern their formation. This strategy is undoubtedly a paradigm shift, which has opened up a path of designing 3D MOFs comprising of flexible counterparts. Exploiting the inherent properties of selected MOFs, I will discuss their application in multi-media iodine capture as an example with mechanistic considerations based on experimental and computational data.



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Biosketch:

Prof. Sanjay Mandal is currently a Professor (HAG) in the department of Chemical Sciences at IISER Mohali. He also served as the Dean Academics and officiating Registrar at IISER Mohali. For two years, he was passionately involved in the Institute's NIRF ranking as the first Nodal Officer. He is the founding Convener of the central X-ray facility at IISER Mohali. As the longest serving Senate member, he continues to contribute to the academic welfare of the Institute. He was a member of Board of Governors and Finance Committee at IISER Mohali. He is a Fellow of Royal Society of Chemistry (FRSC).

He studied at Ramakrishna Mission Narendrapur and IIT Kanpur and received Ph.D. in Chemistry under the guidance of legendary Professor F. Albert Cotton at Texas A&M University, College Station, USA. Prior to joining IISER Mohali in August 2008 as one of the first faculty members, he spent over 20 years in the USA for academic and industry appointments including holding R&D and Management positions in several companies, such as General Electric Company, Dow Corning Corporation, Occidental Chemical Corporation, and Clariant Corporation. His career is equally divided in academia and industry.

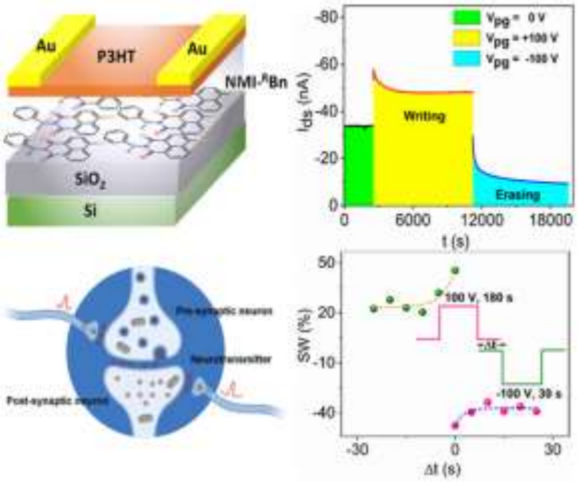
His research interests span across several sub-fields of Chemistry with a special emphasis on Multifunctional Nanomaterials, Crystal Engineering, Organometallic Chemistry and X-ray Crystallography. He teaches a broad range of courses at the BS-MS and PhD level: Basic and Advanced Inorganic/Organometallic Chemistry, Bioinorganic Chemistry, Advanced Industrial Chemistry, Chemical Crystallography, and Supramolecular Chemistry. He is recognized for expertise in Catalysis, Polymer Chemistry, Fluorine Chemistry, X-ray Crystallography, and Six Sigma methodologies. He has published over 270 peer-reviewed articles and reviews in International journals, monographs, and technology reports, and has contributed to over 60 US, Indian and international patents, invention disclosures, trade secrets. Several of his patents were commercialized for products bringing millions of dollars in revenue. At IISER Mohali, he has directed 2 postdocs, 21 PhD students (12 graduated), 9 MS students, and over 50 project/summer students.

T07: Prof. R. Boomi Shankar

Affiliation: IISER PUNE

Title: A Chiral Organic Ferroelectric Exhibiting FeFET and Neuromorphic Applications

Abstract: Molecular ferroelectrics are of tremendous interest due to the ease of their synthesis and simplicity in device fabrication. However, their utility in ferroelectric field effect transistors (*Fe*FETs), memory devices, sensors, and artificial synapses is rarely explored due to the issues related to their band gap mismatch with the metal/organic semiconductor interfaces. Our group has been interested in the design of ferroelectric organic, organic-inorganic hybrid assemblies for energy and electronic applications. To utilize organic ferroelectrics for FET applications, we designed a moderately conjugated enantiomeric organic ferroelectric molecule, 6-bromo-2-(1-phenylethyl)-1H-benzo[de]isoquinoline-1,3(2H)-dione (**NMI-$^{R/S}$Bn**), obtained by introducing the enantiomeric α-methylbenzyl (^{a}Bn) substituents on the naphthalene monoimide (NMI) backbone. As predicted, the **NMI-^{R}Bn** was found to exhibit the FeFET and neuromorphic behaviour on its multi-layer thin film devices. To our knowledge, this is the first time a homochiral single-component organic material has been studied as a memtransistor device.



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Biosketch:

Ramamoorthy Boomi Shankar
Professor
Department of Chemistry
Indian Institute of Science Education and Research (IISER), Pune
Contact Number: 02025908208
E-Mail: boomi@iiserpune.ac.in
Homepage: https://www.boomishankarlab.com

Professor Ramamoorthy Boomishankar obtained his Ph.D. in Chemistry in 2004 from the Indian Institute of Technology (IIT), Kanpur, India. He then took up postdoctoral stints at the University of Illinois at Urbana-Champaign, USA, and the University of Liverpool, UK. He joined IIT, Guwahati as an assistant professor in April 2008. He moved to the Indian Institute of Science Education and Research (IISER), Pune, in 2010 and became a professor in December 2019. His research is focused on the development of polyhedral metal-ligand cages for host-guest studies and chiral separations and on molecular ferro- and piezoelectrics for energy and electronic applications. He is a recipient of the Bronze medal of the Chemical Research Society of India (CRSI) in 2022 and the Science and Technology Award for Research (STAR) from the Science and Engineering Research Board (SERB) in 2021. He is the recipient of the 2024 Annual Alumni Materials Lecture Award of the Chemistry and Physics of Materials Unit (CPMU) at the JNCASR. He is a fellow of the India Chemical Society and a Recipient of the 2024 Silver Star Medal of the Chirantan Rasayan Sanstha (CRS). Currently, he is an Editorial Board Member of the ACS-Inorganic Chemistry.

T08: Prof. Amlan K Roy

Affiliation: IISER KOLKATA

Title: An alternative grid-DFT method for atoms, molecules

Abstract: Density functional theory (DFT) has become a valuable tool for in various branches from organic chemistry to condensed matter physics, over the past few decades. Here, we present an alternative scheme developed in our laboratory in the past few years. Through the use of a pseudopotential Kohn-Sham (KS) DFT framework based on a Cartesian coordinate grid (CCG) and the LCAO-MO ansatz, efforts are made to validate a viable scheme for DFT calculations for small to medium systems. To legitimize its suitability and efficacy, at first, electric response properties, such as dipole moment (μ), static dipole polarizability (α), first hyperpolarizability (β) are computed. Next, we present a purely numerical approach in CCG, to efficiently compute the exact contribution of exchange density in certain types of orbital-dependent density functionals. A Fourier convolution theorem, combined with range-separated Coulomb interaction kernel is invoked. The inspiration for this came from a semi-numerical approach where the assessment of electrostatic potential determined the rate. Its success further leads to a systematic self-consistent approach from first principles, which is desirable in the development of optimally tuned range-separated hybrid and hyper functionals. We then go over a quick, alternate time-independent DFT method using the "adiabatic connection theorem" and the "viral theorem" to compute single-particle excitation energies. Optical gaps in organic chromophores, dyes, linear/non-linear PAHs, charge transfer complexes are accurately simulated. In addition to investigating the time-independent regime, we provide a novel method towards RT-TDDFT using time-dependent KS equations based on an adiabatic eigenstate subspace (AES) procedure. To implement the approximate TD propagator in AES, it provides a second-order split operator approach. The majority of the TDKS matrix elements are computed directly in CCG. The practicality of this suggested route is ensured by comparison with existing theoretical conclusions. In summary, CCG-DFT is demonstrated to be an effective path for a variety of real-world applications in electronic systems.

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12. A. Ghosal and A. K. Roy, *Mol. Phys.* **120**, e1983056 (2022).

13. R. Roy, A. Ghosal, and A. K. Roy, *J. Phys. Chem. A* **126,** 1448 (2022).

Bio sketch:

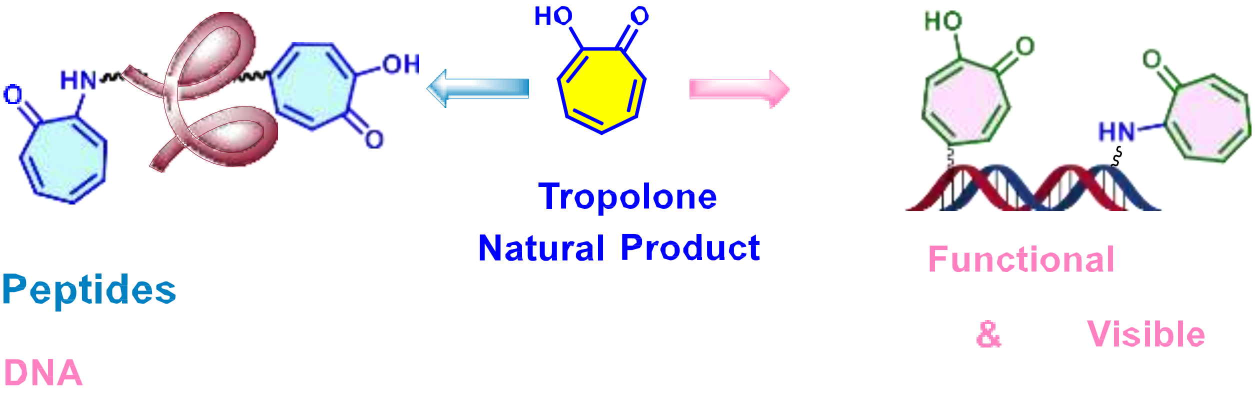
Dr. Amlan. K. Roy completed his PhD in theoretical chemistry from Panjab University, in India. Later he pursued his post-doctoral research in a number of places in North America, such as University of New Brunswick (Fredericton, Canada), University of Kansas (Lawrence, USA), University of California (Los Angeles, USA), University of Florida (Quantum Theory Project). His primary research interest is to develop methods for electronic structure and dynamics of many-electron systems, within the broad domain of density functional framework. Some other interests include quantum confinement and quantum information theory. Presently he is a professor at IISER Kolkata, Chemistry department. He has published more than hundred research papers and book chapters in reputed journals. He has been serving as a reviewer in many renowned journals. His biography has been included in 63rd Edition of Marquis Who's Who in America, 2009. In 2012 he has edited a book entitled "Theoretical and Computational Developments in Modern Density Functional Theory". In 2024, he has edited another book entitled "A closer look at the Hydrogen atom

T09: Prof. Nagendra Kumar Sharma

Affiliation: NISER BHUBANESWAR

Title: Synthesis and Evaluation of Non-benzenoid Scaffold (Tropolone) Incorporated Biomacromolecules (Peptides and DNA)

Abstract: The aromatic residues of biomacromolecules (Aromatic amino acid/Nucleic acid) are derived only from the benzenoid aromatic system. However, non-benenoid scaffolds (Tropolone and Tropone) are also occurred as constituents of various natural products.[1] Some of these natural products exhibit strong bioactivities and are considered therapeutic agents. Structurally, tropolone is an excellent natural chromophore possessing unique inter-/intramolecular hydrogen-bonding ability. Tropolone also forms complex structure divalent metal ions, mainly for Cu(II). biomacromolecules. Recently, we have explored *N*-troponyl-amino acid/peptide derivatives that exhibit interesting structural and functional properties including anticancer activities.[3] Importantly, we have successfully incorporated troponyl-residue into DNA oligonucleotides and explored their biophysical/photophysical properties.[4]



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3. *N K Sharma et. al. (a)* ChemBioChem, **2019**, *20*, 1-10. (b) ChemBioChem, **2023**, *24*, 1e202200732.

Bio sketch:

Dr. Nagendra K. Sharma

Associate Professor,
School of Chemical Science, National Institute of
Science Education and Research(NISER),
Bhubaneswar, (Odisha) India

Research Interest: Chemical synthesis of biomolecules (Amino acid and Nucleic Acid DNA/RNA).

Education

2012-Continue: Faculty (Assistant Profeessor, Reader-F, Associate Professor) NISER Bhubaneswar

2009-2012: Visiting Faculty, NISER Bhubaneswar

2006-2009 Post. Doc.- Department of Chemistry, University of Utah, Salt Lake City, Utah (USA) (Mentor: Prof. Dale C. Poulter)

2000-2006 Ph.D.- National Chemical Laboratory (NCL)- Pune & (University of Pune)- Maharashtra (Mentor: Prof. K. N. Ganesh)
1999 M.Sc (Spl. Organic Chemistry).- University of Delhi, Delhi **1997 B.Sc (Honours):** University of Delhi, Delhi

T10: Prof. Padmabati Mondal

Affiliation: IISER TIRUPATI

Title: Understanding Serotonin-Receptor Interactions, Binding and Stability via Molecular Dynamics Simulations: Key Residues for non-covalent Interactions and Signal Transduction

Abstract: Serotonin-receptor binding is the key to several neurological and biological processes, including mood, sleep, hunger, cognition, learning, and memory. Here I will be talking about a molecular dynamics simulation study to understand the serotonin and G-protein-coupled receptor (5-HT$_{1B}$R) interactions, binding and stability via non-covalent interactions as well as signal transduction pathway upon serotonin binding. The order parameters defined based on centre of mass distance and angle between surface normals provide qualitative information about stacking interactions between serotonin and aromatic amino acid residues in the binding site. The electrostatic interactions between serotonin and receptor were detected based on bond distance analysis and frustration analysis. An end-point free energy calculation method determines the stability of the 5-HT$_{1B}$ R due to serotonin binding. The single-point mutation of the aromatic and polar/charged amino acid residues on the binding sites and the binding free energy calculation validate the importance of these residues in the stability of the serotonin-receptor complex. Principal component analysis indicates that the serotonin-bound 5-HT$_{1B}$R is more stabilized than the apo-receptor in dynamic changes. The difference dynamic cross-correlations map shows the correlation between the transmembranes and mini-G$_o$, indicating signal transduction between mini-G$_o$ and the receptor. Allosteric pathway analysis reveals the key nodes for signal transduction in 5-HT$_{1B}$R. These results provide valuable insights into the study of signal transduction pathways and mutagenesis to regulate the functionality of the complex. The developed protocols can be applied to study local non-covalent interactions and long-range allosteric communications in any protein-ligand system for computer-aided drug design.

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2) P. Mondal; *RSC Adv.* 2020, 10, 37995-38003

3) A. Verma; P. Mondal; *BioPhys. Chem., 2025, 318, 107386*

Bio-Sketch:

Name: Padmabati Mondal

Present Position: Assistant Professor, Chemistry (Since February, 2019)

Affiliation: Indian Institute of Science

Education and Research (IISER) Tirupati, Andhra Pradesh, India

Research Interest: Theoretical and Computational Chemistry

(Excited state quantum chemistry and multiscale simulation)

PhD: Technical University of Munich, Germany

PostDoc: Goethe University Frankfurt, Germany

University of Basel, Switzerland

Aix-Marseille University, France

E-Mail: padmabati.mondal@iisertirupati.ac.in

Homepage: https://www.iisertirupati.ac.in/faculty-details/?faculty_id=Che-20&id=2376 https://padmabatimondal.weebly.com/

T11: Prof. Ahanjit Bhattacharya

Affiliation: IISER BHOPAL

Title: Applications of functional lipid assemblies in bottom-up construction of artificial cellular systems

Abstract: Compartmentalization is a defining feature of all forms of life. Processes like signalling, transport, and biosynthesis take place in cells through the interplay between structure and dynamics of cellular membranes. Amphiphilic lipid molecules are the primary building blocks of cellular membrane compartments. Here we take a bottom-up approach to develop a fundamental understanding of the role of lipid membranes in cellular compartmentalization. Various lipid architectures were used to build functional models (artificial cells and organelles) of the membranous structures found in cells. We utilized giant vesicles to recapitulate the basic membrane-bound structure of cells.[1,2] To model membrane-rich organelles such as the endoplasmic reticulum, we described a novel bicontinuous lipid sponge phase lipid droplet system.[3,4] With their nanoporous structure consisting of an interconnected network of bilayers, lipid sponge droplets can sequester hydrophobic and hydrophilic molecules in a programmable manner at concentrations comparable to that in cells. We further explored the structure-function relationships in the amphiphiles that form sponge phase and obtained a physical model for the observed behaviour. In summary, bottom-up development of artificial cells and organelles is a highly creative pursuit which leads to the discovery of new novel functional materials, emergent phenomena, and research tools.

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Bio sketch:

Ahanjit Bhattacharya is an Assistant Professor of Chemistry at the Indian Institute of Science Education and Research, Bhopal. He is the Principal Investigator of the Chemical Synthetic Biology Laboratory. Ahanjit graduated in Chemistry with minor in Biotechnology from IIT Kharagpur as the Prime Minister of India Gold Medalist (2014), Ahanjit carried out his doctoral research at the University of California San Diego under the guidance of Neal Devaraj. Here, he worked on designing artificial cellular systems from fundamental chemical and biochemical building blocks. Ahanjit's major accomplishments are the development of programmable lipid compartments as artificial cells and organelles and designing minimal biochemical strategies for synthesis of membrane-forming lipids. His experience with lipids and soft matter physics inspired him to gain expertise around membrane biophysics during postdoctoral tenure in the lab of Steven Boxer. At Stanford, Ahanjit has worked on biophysical mechanisms of fusion of enveloped viruses like influenza. He has also studied structure-function relationships in archaeal bipolar lipids to shed light on cellular physiology of extremophilic archaea. His association with the Stanford Center for Innovation in Global Health as a postdoctoral affiliate inspired him to develop low-cost solutions to human health problems in the developing world. Ahanjit’s research work led to several awards including his recognition as one of the CAS Future Leaders Top 100 (2024), and Reaxys PhD Prize Finalists (2020). Ahanjit enjoys teaching and received the Postdoc Teaching Certificate from Stanford in recognition of his comprehensive teaching training and practice. Ahanjit is passionate about communicating science and making it a transformational force for betterment of society and humanity.

T12: Prof. Sanchita Sengupta

Affiliation: IISER MOHALI

Title: Multichromophoric Light-Harvesting Systems and Their Composites for Photocatalytic Hydrogen Evolution and Organic Transformations

Abstract: Homogeneous and heterogenous photocatalysis provide access to sustainable and alternative energy source such as hydrogen (H_2) and facile synthetic routes for organic compounds under benign experimental conditions. Here, the synthesis of organic (multi)chromophoric systems and their photophysical and electrochemical characterization will be presented followed by their composite formation with g-C_3N_4.[1-4] The chromophore-g-C_3N_4 composites were prepared via both calcination and p-p stacking to form *in-situ* and *ex-situ* composites.[1] These composites were utilized as heterogeneous photocatalysts for H_2 evolution and achieved a 10-fold enhancement in H_2 evolution compared to only g-C_3N_4 and facilitated photocatalytic oxidative amidation of aldehydes and amines with high yields (80%).[1,2] Furthermore, a multichromophoric Iridium-based perylene monoanhydride compound was utilized as a homogeneous photocatalyst that efficiently catalyzed the synthesis of tetrahydroquinolines from malemides and *N*, *N*-dimethylaniline via sp^3 C−H bond functionalization, yielding products with up to 83% yields.[3] Finally, a few strategic design aspects of chromophores for homogeneous and heterogeneous photocatalysts for a variety of organic transformations will be discussed.[1-4]

Keywords: Photocatalyst; Chromophore; H_2 evolution, Organic Transformation; Heterogeneous photocatalyst

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4. Unpublished results.

Bio sketch:

Sanchita Sengupta

Designation: Associate Professor

Affiliation: Department of Chemical Sciences
Indian Institute of Science Education and Research (IISER) Mohali

Email: sanchita@iisermohali.ac.in
Webpage: http://www.iisermohali.ac.in/faculty/dcs/sanchita

Education: Ph.D. - University of Würzburg (Germany)
M.Sc.- Indian Institute of Technology (IIT) Kanpur

Employment:
Associate Professor (2023-present); Assistant Professor (2017-23) at IISER Mohali

Brief description of research: Dr. Sanchita Sengupta received her M.Sc. (Chemistry) from Indian Institute of Technology Kanpur and Ph.D. from University of Würzburg, Germany. Her postdoctoral stays were at Univ. Würzburg, Technical University Delft, the Netherlands and INSPIRE faculty fellowship at Indian Institute of Science, Bangalore prior to joining IISER Mohali. Research in the group is directed towards development and characterization of π-conjugated organic molecules to control their excited state properties for specific applications (fluorescence ratiometric sensing, optoelectronics and photocatalysis), particularly as following themes: i) Multichromophoric light harvesting (LH) antenna and macrocycles for energy transfer and their utilization as multi-stimuli responsive sensors; ii) Donor-acceptor (D-A) rotors as multifunctional sensors (iii) (Twisted) D-A conjugates for efficient charge transport and thermally activated delayed fluorescence (TADF) materials; (iv) applications of above molecules as metal-free visible and near infrared light photocatalysts for organic transformations and hydrogen evolution. Dr. Sengupta is a recipient of Chemical Research Society of India (CRSI) Young Scientist Award 2022 and serves as early career advisory board (ECAB) member of the journals Organic Chemistry Frontiers (RSC) and ChemistrySelect (Wiley).

T13: Prof. Subhajit Roychowdhury

Affiliation: IISER BHOPAL

Title: Evidence of Ferroelectric Distortions in Topological Crystalline Insulators via Transverse Thermoelectric Measurements

Abstract: The transverse thermoelectric (Nernst) effect is a powerful probe for studying the electronic and structural properties of materials.[1] In this study, we employ transverse thermoelectric measurements to investigate the ferroelectric distortion in the topological crystalline insulator (TCI) $Pb_{0.60}Sn_{0.40}Te$, a compound derived from PbTe and SnTe, known for their exceptional thermoelectric performance and distinct ferroelectric properties. By leveraging Nernst measurements, we provide direct evidence of ferroelectric distortion in this TCI, corroborated by Shubnikov–de Haas quantum oscillations that confirm the presence of two topologically non-trivial Fermi pockets. Density functional theory (DFT) calculations show that these pockets to originate from the L and T points in the Brillouin zone of the distorted structure within the TCI phase. Raman spectroscopy further identifies a structural phase transition below 50 K, consistent with the quantum oscillation observations. These findings underscore the potential of transverse thermoelectric measurements in unveiling ferroelectric distortions and their role in modulating topological quantum states, opening new directions for research into the synergy between ferroelectricity and topological phases.

References:

S. Roychowdhury, A. M. Ochs, S. N. Guin, K Samanta, J Noky, C. Shekhar, M. G. Vergniory, J. E. Goldberger, C. Felser, *Adv. Mater.,* **2022**, *34*, 2201350

Bio sketch:

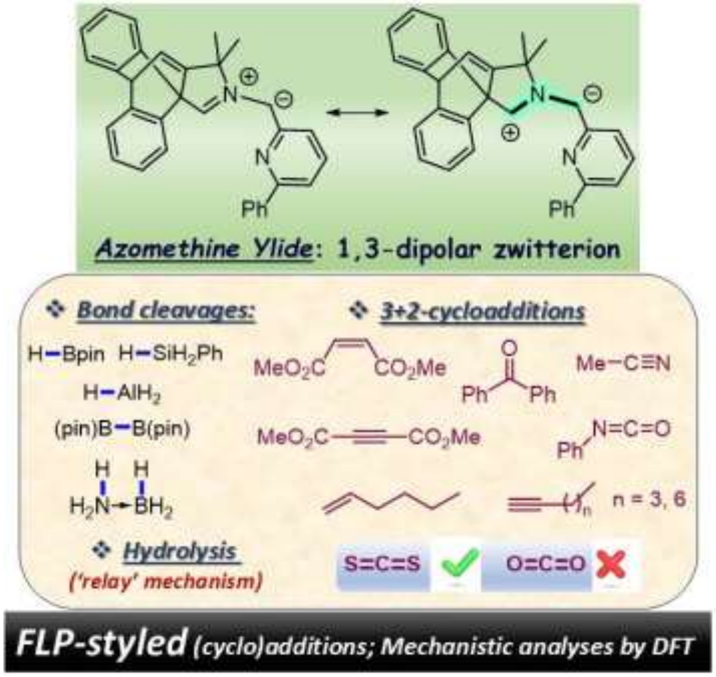
Dr. Subhajit Roychowdhury received his Ph.D. from Jawaharlal Nehru Centre for Advanced Scientific Research, India in 2019, worked as a Research Associate at JNCASR for some time (August 2019 – January 2020) and then became a Postdoctoral Research Fellow and Humboldt Fellow in Max Planck Institute for Chemical Physics of Solids, Dresden, Germany (February 2020 – February 2024). He is currently working as Assistant Professor at IISER Bhopal. His research interests include the synthesis of single crystals of topological quantum materials, magneto-thermoelectric effect for energy harvesting, topological quantum materials for studying the magnetic, electrical, and thermal transport properties, high-temperature Nernst effect.

T14: Prof. Debabrata Mukherjee

Affiliation: IISER KOLKATA

Title: FLP-like (Cyclo)addition of Small Organic Molecules to a Stable Azomethine Ylide

Abstract: Azomethine ylides are 1,3-dipolar zwitterions typically used for constructing N-heterocycles by 3+2- cycloaddition reactions. We report here a pyridyl-tethered isolable azomethine ylide (**AY**) that activates a series of H□E bonds (E = B, Si, Al, O) in FLP-like fashion. The reactions are probed mechanistically by DFT calculations and each case appears to be distinct from others. While the HBpin activation is stepwise, the same of PhSiH3 is concerted. The AlH3 activation is also stepwise but takes place across the 1,5-(C^{+}/$N^{□}$) dipole. The hydrolysis of **AY** fits better with a 'relay' mechanism with two H2O molecules working in tandem. The B□B bond of B2pin2 is also cleaved but in an intriguingly different way, by delivering both the Bpin moieties at the carbenic site. Though the coveted H2 activation fails, a transfer hydrogenation of **AY** by NH3•BH3 is readily achieved. **AY** also undergoes cycloadditions with various dipolarophiles including unactivated alkene and alkynes. In this regard, **AY** makes an interesting distinction between CO2 and CS2 by staying inert to the former but easily cycloadding the latter. DFT analysis justifies this dichotomy by showing the cycloaddition of CO2 as thermodynamically disfavored.



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3. S. Baguli, S. Sarkar, D. Mallick, D. Mukherjee, *ChemRxiv* **2025**, *DOI:* 10.26434/chemrxiv-2024-b2r6c.

Bio sketch:

T15: Prof. Bishnu Prasad Biswal

Affiliation: NISER Bhubaneswar

Title: Nanoparticle Organic Networks: A New Class of Functional Materials

Abstract: Reticular chemistry has significantly expanded materials science, yielding various frameworks such as metal-organic frameworks (MOFs), covalent organic frameworks (COFs), etc.[1] The broad utility of these materials stems from their remarkable properties, including high crystallinity, tunable metrics, organic functionality, and intrinsic porosities. In particular, MOFs consist of high-valent metal ion/cluster nodes connected by organic mono/multi-topic linkers.[2] However, the use of metals in zero oxidation state (O.S) as nodes to construct a reticulated structure is anticipated to enhance the material's optoelectronic and catalytic characteristics, akin to the observed properties of metal nanoparticles (MNPs). In my talk, I will discuss one of our recent works, wherein we designed and synthesized a novel network structure of MNPs [nanoparticle organic networks (NONs)]. The covalent linkage of zero-valent MNP nodes and bifunctional organic struts resulted in the NONs employing a sustainable mechanochemical approach.[3],[4] In addition, capitalizing on the excellent optoelectronics of MNPs, the scope of NONs as semiconducting composite materials for transistor device fabrication will be covered. The preliminary results showed an enhancement of the in-plane charge transport mobility and a stupendous increase in photoresponsivity upon incorporating NONs into the semiconducting polymer matrix. Towards future prospects, these precontrived networks of MNPs with covalently bonded organic linkers open up a general strategy for developing a new class of composite semiconductors for high-performance optoelectronic devices.

References:

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Bio sketch:

Dr. Biswal is currently working as Reader-F at the School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha since July 2023. Prior to this position, he served as an Assistiant Professor at the same institute from Dec. 2020 – June 2023. He received a Ph.D. in the year 2017 from Academy of Scientific and Innovative Research, CSIR-National Chemical Laboratory, Pune; Master of Science (2010) and Bachelor of Science (2008) in Chemistry from Utkal University, Bhubaneswar, Odisha. He was an Alexander von Humboldt fellow at Max-Planck-Institute of Solid-State Research, Stuttgart (Dec. 2017 - Aug. 2020) and Institute Post-doc fellow at Technical University Dresden, Germany (Sept. 2016 - Sept. 2017). Dr. Biswal has expertise in the field of physical and materials chemistry. His research is the interdisciplinary blending of experimental chemistry, material science, and engineering. His group at NISER Bhubaneswar is developing advanced reticular materials and membranes for sustainable applications.Dr. Biswal so far published 50 peer-reviewed international research papers, review articles and book

chapters that have been cited over 9400 times with an H-index of 33 (as per Google Scholar).

T16: Prof. Hirendra N. Ghosh

Affiliation: NISER Bhubaneswar

Title: Ultrafast Plasmon Dynamics in Non-stoichiometric Near Infrared Active Semiconductor Nanocrystals

Abstract: Surface plasmon resonance (SPR) in nanomaterials (NMs) facilitates the generation of hot carrier (electron-hole) through plasmon decay and has garnered substantial and increasing attention over the past two decades. Plasmonic NMs have numerous unique properties like high extinction co-efficient, long-range light absorption (Visible to IR), cost-effectiveness and easy to manipulate their physical properties. These attributes render them highly promising materials for multiple applications, including photocatalysis, photodetectors, nanophotonics and photothermal therapy etc. In the present talk we will discuss ultrafast plasmon dynamics in non-stoichiometric $Cu_{2-x}Y$ (Y=S, Se) semiconductor nanocrystals (NCs). Transient spectra exhibit extended absorption span over entire infrared region, which is plasmon excitation or hot hole transition within the valence band of NC. Following transient kinetics we have monitored hole-hole, hole-phonon and phonon-phonon scattering, respectively. We have also demonstrated dynamics of hot hole delocalization and transfer dynamics in a p-n hetero-junction consisting of $Cu_{2-x}Se$ and CdSe/CuInSe. Finally, we have successfully unraveled the process of plasmon-induced hot hole extraction, whereby hot holes are transferred from gold (Au) to $Cu_{2-x}Se$, within the framework of dual plasmonic hybrid nanocrystals (HNCs) comprising Au@$Cu_{2-x}Se$. These findings will open up a new avenue for harvesting visible to near infrared photon for the development of modern solar cells, photodetector and fast nanophotonic device application.

References

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7. Kharbanda, N.; Sachdeva, M.; Ghorai, N.; Kaur, A.; Kumar, V.; Ghosh, H.N. *J. Phys. Chem Lett*, **2024,** *15*, 5056-5062.
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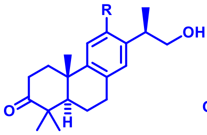
Bio sketch:

T17: Prof. Rajendar Goreti

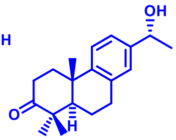
Affiliation: IISER Thiruvananthapuram

Title: Enantioselective Approaches for the Structure Assignment of Abietane Diterpenoid

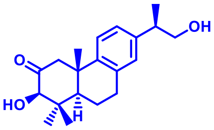
Abstract: Aromatic abietanes are important diterpenoids found in various terrestrial plants and are of significant interest in pharmacology due to their diverse biological activities. These compounds typically possess a common [6-6-6] tricyclic 20-carbon framework with an aromatic C-ring, exhibiting distinct oxidation states across the A, B, and C ring systems. Euolutchuols, isolophonthins, nagiol, and ferruginols have been isolated from different plant species, including the roots of *Euonymus lutchuensis*, the leaves of *Isodon lophanthoides var. gerardianus*, and *Podocarpus nagi*. These diterpenoids were synthesized directly through biomimetic cationic polyene cyclization of an epoxy polyene. Various enantio- and diastereoselective oxidation reactions have been employed to generate structurally diverse natural diterpenoids. Different synthetic isomers were prepared and their structures were assigned and revised using NMR spectroscopy and single-crystal X-ray analysis of, providing valuable insights into the structural features of these bioactive compounds.



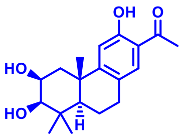
R = H; Euolutchuol A
R = OH; Euolutchuol B
(assigned)



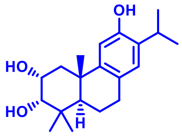
Euolutchuol C
(assigned)



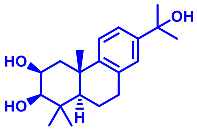
Euolutchuol D
(assigned)



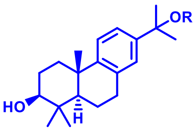
nagiol
(revised)



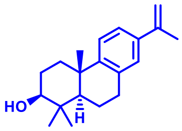
2,3-dihydoxy ferruginol
(revised)



Isolophanthin E
(revised)



R = H; Isolophanthin A
R =Me; Isolophanthin B
(reported)



3b-hydroxy-abieta-8,
11,13,15-tetraene

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Bio sketch:

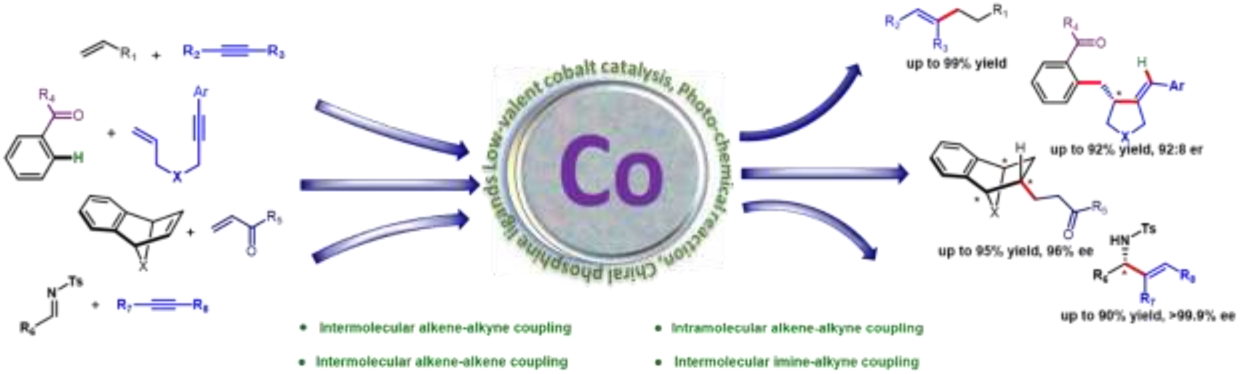
Dr. Goreti Rajendar earned his PhD in 2012 from IICT Hyderabad under the guidance of Dr. J. S. Yadav. He then pursued postdoctoral research in Prof. E. J. Corey's group at Harvard University, Cambridge, USA. In 2016, he commenced his independent academic career at the Indian Institute of Science Education and Research (IISER) Thiruvananthapuram. His research focuses on asymmetric organic synthesis, encompassing the total synthesis of natural products and bioactive small molecules, development of novel synthetic methods, and the design of new chiral auxiliaries and catalyst systems.

T18: Prof. Biplab Maji

Affiliation: IISER KOLKATA

Title: Asymmetric Reductive Coupling Reactions Catalyzed by Cobalt Diphosphine Complexes

Abstract: Over the past few decades, low-valent metal-catalyzed reductive coupling reactions have been one of the most used strategies to pull off new carbon-carbon bonds.1 Initially started with precious metal-based reductive coupling, soon replaced by the more abundant and less expensive early transition metals. In this idea, complex organic transformation can be achieved by reducing a metal from a higher oxidation state to its more reactive lower oxidation state. The reduction can be carried through employing a metal reductant or using milder conditions of photo-redox catalysis.2 In this context, cobalt, as an early transition metal, was found to have great potential for various reductive coupling reactions.3 Our group utilizes low-valent cobalt catalysis with different phosphine ligands to perform intermolecular alkene-alkyne coupling,4 intramolecular alkene-alkyne coupling,5 alkene-alkene coupling,6 and imine-alkyne coupling7 with excellent chemo, regio, and enantio stereoselectivity (Figure 1). These methodologies showed excellent substrate scope compatibility with a broad functional group tolerance. Further mechanistic transformations were performed to elucidate the mechanistic hypothesis.



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Bio sketch:

1987: Born, Howrah, India

2007: B.Sc. University of Calcutta (Chemistry Hons.)

2009: M.Sc. Indian Institute of Technology Kanpur (Chemistry)

2012: PhD Ludwig Maximillan Universität Munich, Supervisor: Prof. Herbert Mayr

2013-2015: Postdoc: Chubu University, Mentor: Prof. Hisashi Yamamoto

2016: Alexander von Humboldt fellow: Westfälische Wilhelms-Universität Münster, Mentor: Prof. Frank Glorius

2016-2021: Assistant Professor, Indian Institute of Science Education and Research Kolkata

2021-: Associate Professor, Indian Institute of Science Education and Research Kolkata

Research focus: Organic synthesis, catalysis, and mechanistic studies.

Awards:

2024: Associate of the West Bengal Academy of Science & Technology (WAST)

2021: "2021 Young Investigator Award ", Sponsored by Molecules

2021: Merck Young Scientist Award (runner-up) in Chemical Science

2021: INSA Medal for Young Scientists

2021: Associate of the Indian Academy of Sciences (IASc)

2020: NASI-Young Scientist Platinum Jubilee Award (2020) in Chemical Sciences

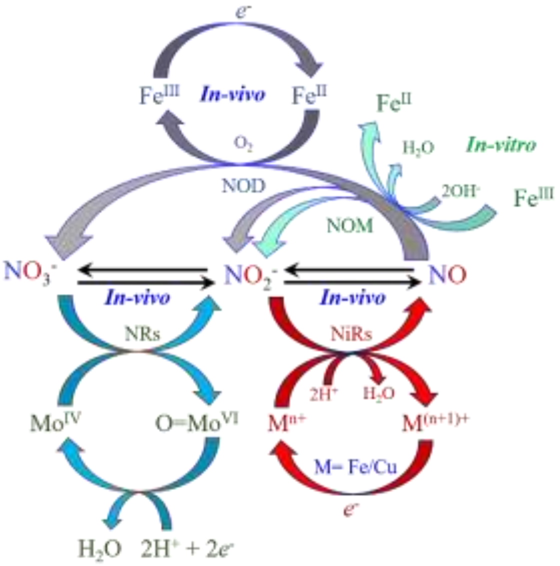
2019: Thieme Journal Award

T19: Prof. Pankaj Kumar Koli

Affiliation: IISER TIRUPATI

Title: Biomimetic Modelling of Interconversion of Nitric Oxide and its derivatives

Abstract: Nitric oxide (NO) is a crucial molecule involved in numerous physiological processes, including neurotransmission, vascular regulation, platelet disaggregation, and immune responses to various infections.[1] To ensure the maintenance of optimal NO levels, the activity of key enzymes such as nitrate reductase (NR) and nitrite reductase (NiR) plays a vital role.[2] While NO synthase (NOS)[3] enzymes are available for NO biosynthesis, NO Dioxygenase (NOD) enzymes convert NO to biologically benign NO_3^- if overproduced. NR catalytically transforms the NO_3^- to NO_2^- via the O-atom transfer (OAT) reaction via Mo/W-based enzymes. Meanwhile, NiR enzymes catalyze the conversion of NO_2^- to NO by using acid (H^+).[2] Biological dysfunction may lead to NO overproduction, which is usually converted to NO_3^- in the presence of NOD enzymes. This regular interconversion helps maintain biological NO homeostasis. This report will explain the reduction of NO_2^- to NO via acid-induced reaction[4] and OAT chemistry at Co[5]/Fe/Cu centers. In addition, it will also provide a brief report on NO oxidation reaction of $\{CoNO\}^8$ to understand the mechanistic aspects of these reactions.[6] A new pathway for NiR enzyme activity was observed with one equivalent proton (H^+) generating M-NOs (or NO generation) with H_2O_2 (which further decomposes to H_2O). In addition, VCl_3-induced NO_3^-/NO_2^- reduction was also confirmed on Co-center. Further, to complete the NO-biological cycle, we reacted the M-NO with OH^-/O^{2-}, showing the formation of the M^{n+}-NO_2^-, in contrast to one of our previous reports of $\{CoNO\}^8$ with O_2, leading the generation of Co^{II}-NO_3^- (NOD product).[7]



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Bio sketch:

Dr. Pankaj Kumar Koli completed his Ph.D. in 2013 from the Indian Institute of Technology, Guwahati. He was a WCU Postdoctoral fellow at the Center for Biomimetic Systems, Department of Chemistry and Bioinspired Science, Ewha Womans University from 2013-2016. In 2017, he joined M. M. University, India, to work as an assistant professor in the Department of Chemistry from 2016-2017. In the same year, he started his independent career at IISER Tirupati. Presently, he has been an associate professor at the institute since 2023. Dr. Koli works on intermediates biologically important small molecule activation, i.e., O_2, NO, CO, CO_2, and H_2S, etc., with transition metal ions to mimic in-vivo enzymatic systems responsible for various biological reactions and working to develop the probes for their detection. Also, he is working on biomimetic modeling and intermediates mimic and stabilize, i.e., Metal-Oxo /-Peroxo /-Superoxo, Metal-Nitrosyl, and Metal-Carbonyl. His research experience helped him to secure several research grants from SERB (3), GAIL, AvH (Humboldt Experienced Research Awards, 2021-2024), DAAD (Experienced Research Award, 2021), and also mentoring a project for WISE-DST Scientist (2024-2027).

T20: Prof. Himansu S Biswal

Affiliation: NISER BHUBANESWAR

Title: Can Thioamides be the Potential Surrogates of Amides?

Abstract: The replacement of carbonyl oxygen with sulfur in thioamides leads to distinct reactivity and physical properties compared to amides. This substitution weakens resonance stabilization, creates a more polarizable C=S bond, and fundamentally alters molecular behavior. This presentation explores the potential of thioamides as amide surrogates, focusing on how these structural changes impact aromaticity, hydrogen bonding, fluorescence energy transfer

(FRET), and photo-induced electron transfer (PET). Utilizing advanced spectroscopic techniques, including supersonic-jet spectroscopy, NMR, and fluorescence up-conversion spectroscopy, we will delve into the molecular-level differences between these classes of compounds. We will demonstrate how these differences can make thioamides viable replacements of amides in specific applications. Finally, we will provide a brief overview of the sophisticated instrumentation required for these detailed molecular studies, highlighting the power of spectroscopy in unraveling the intricacies of chemical structure and function.

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Bio sketch :

T21: Prof. Angshuman Nag

Affiliation: IISER PUNE

Title: Short-Wave Infrared Emitting Halide Perovskites

Abstract: Short-wave infrared (SWIR) radiation, ranging from 700 to 1700 nm, is important for applications in bio-imaging, security camera, food inspection, remote-sensing, and optical fibre communication. Epitaxially grown III-V semiconductors are common choice for SWIR light emitting diodes (LEDs), but with limitations in mass production and high expense. Therefore, the development of suitable SWIR emitters, particularly the broadband ones, remains a significant challenge. This talk covers designing broadband SWIR emitters by doping metal halide double perovskites like $Cs_2NaInCl_6$. Such a host offers suitable octahedral coordination for potential SWIR-emitting dopants and is both stable and environmentally benign. Doping lanthanides such as Yb and Er produces sharp SWIR radiation at 990 nm and 1540 nm, respectively, via f-f transitions.[1,2] But the spectral width of *f-f* transitions is typically narrow. So, for achieving broadband SWIR emission, we doped transition metal ions with *d-d* transitions. Broad dual emitter covering white-light emission and SWIR emission was achieved by codoping Bi^{3+} and Cr^{3+}.[3] Thereafter, we achieved ultrabroad SWIR emitters with unprecedented FWHM of ~450 nm, by doping W or Mo in $Cs_2Na_{0.95}Ag_{0.5}BiCl_6$ double perovskite.[4] Subsequently, we fabricated prototype phosphor-converted LED panels with over 100 LEDs, demonstrating their capabilities for SWIR imaging and food freshness inspection.

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Bio sketch :

Angshuman Nag is a Professor of Chemistry at IISER Pune, India. He did his Ph. D. from IISc Bangalore in 2009, and subsequently completed two terms of postdoctoral research at JNCASR Bangalore and the University of Chicago. He started his research group at IISER Pune as a Ramanujan Fellow in the year 2012. His research is focused on developing novel semiconductors like halide perovskites and colloidal quantum dots for optoelectronic applications**.**

T22: Prof. Sureshkumar Devarajulu

Affiliation: IISER KOLKATA

Title: How Distal is Distal C(sp3)–H Activation?

Abstract: A mild, redox-neutral, and transition-metal-free methodology for tandem perfluoroalkylation and remote C(*sp*³)–H alkylation of terminal alkenes has been developed using organophotocatalysis. This approach demonstrates exceptional chemo- and regioselectivity, enabling the precise difunctionalization of unactivated alkenes at various distances, including the 1,10, 1,14, 1,11, 1,7, and 1,6-positions. A notable highlight of this work is the unique radical translocation between secondary C(*sp*³) centers with comparable bond dissociation energies, representing a significant advancement in radical-based synthetic strategies. Additionally, the study introduces a tandem process integrating trifluoromethylation, 5-exo-trig cyclization, 1,5-radical translocation, and C(*sp*³)–H alkylation on 1,6-dialkenes. A key breakthrough lies in the multi-component, transition-metal-free tandem strategy for synthesizing highly substituted cyclopentane derivatives. The synthetic utility of this methodology is further highlighted by its scalability and the facile transformation of products into valuable functional groups, underscoring the broad applicability and versatility of this approach.

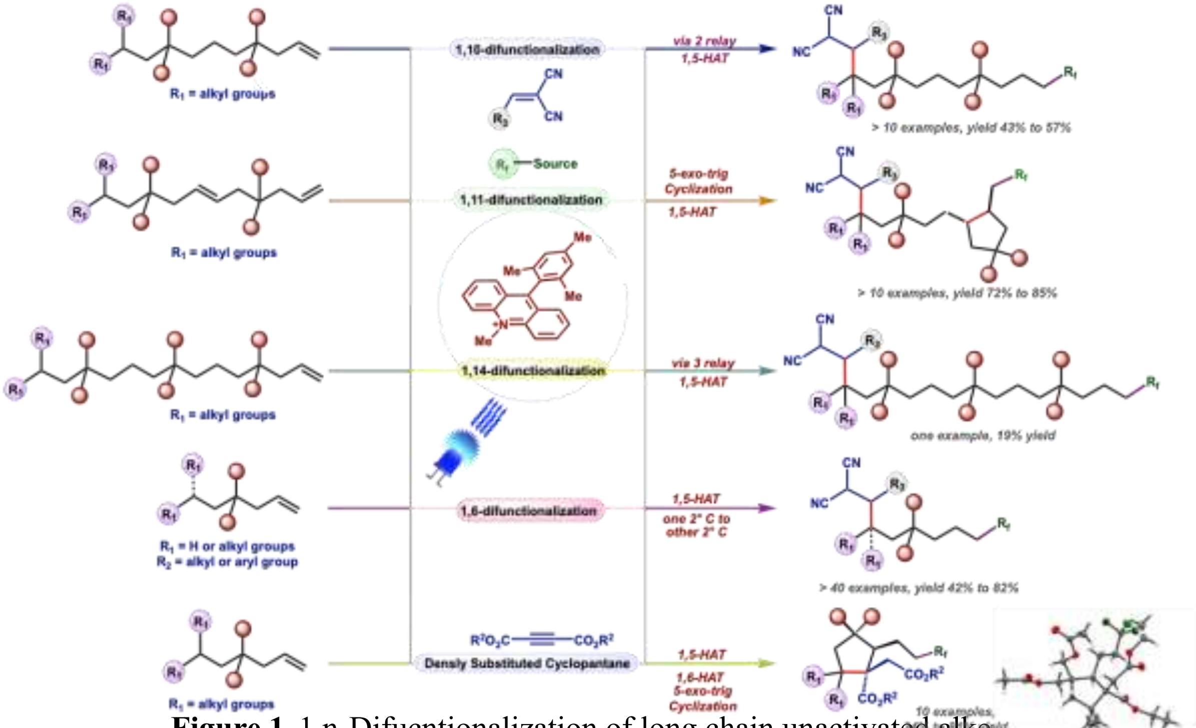

Figure 1. 1,n-Difucntionalization of long chain unactivated alke

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Bio sketch :

Devarajulu Sureshkumar completed his B. Sc. in Chemistry and M. Sc. in Organic Chemistry at the University of Madras. He earned his Ph.D. in 2007 under the supervision of Prof. S. Chandrasekaran, Department of Organic Chemistry, IISc Bangalore. From 2008 to 2010, he was an AvH postdoctoral fellow, working with Dr. Martin Klussman in Prof. Benjamin List's group at the Max-Planck-Institute for Kohlenforschung, Germany. He then undertook a short postdoctoral associate position with Prof. Wilhelm Boland at the Max-Planck-Institute for Chemical Ecology in Jena, Germany, before moving to Japan as a JSPS fellow. There, he worked with Prof. Masakatsu Shibasaki at the Institute of Microbial Chemistry in Tokyo (2010-2015). He joined the IISER Kolkata as a faculty in the Department of Chemical Sciences in February 2015. His research focuses on visible-light-mediated photocatalysis for C–C bond-breaking and forming and fluorination reactions through C(sp^3)–H functionalization.

Significant Awards/Achievements:

Early Carrier Research Award-2017 from SERB, Government of India.

Ramanujan Fellowship-2016 from SERB/DST, Government of India.

JSPS Fellowship-201 for Foreign Researchers (Pathway to University Positions in Japan).

JSPS Fellowship-2011 at Institute of Microbial Chemistry, Tokyo, Japan.

AvH Fellowship-2008 at Max-Planck Institute for Khölenforschung, Germany.

Representative Publications:

1. Visible-Light Driven Synthesis of Vinyl Amines without Photocatalyst. Pal, K.; Das, D.; Ghosh, K. G.; Sureshkumar. D. *J. Org. Chem.* **2024**, *89*, 15317-15324
2. Photocatalyzed Direct C(sp^3)–H Alkenylation of Unactivated Alkanes *via* Tandem C–C Activation of Cyclopropenes. Biswas. S.; Das, D.; Pal, K.; Chandu, P.; Sureshkumar. D. *J. Org. Chem.* **2024**, *89*, 12421-12431.
3. Photoredox Cross Dehydrogenative C(sp^2)–C(sp^3) Coupling of Heteroarenes with Secondary Amines through 1,5-HAT. Srinivasu, V.; Patanaik, S.; Sureshkumar, D. *Chem. Commun*. **2024**, *60*, 9757-9760.

T23: Prof. Malay Rana

Affiliation: IISER BERHAMPUR

Title: Amendments to MOF-5 and UiO-66 for Improved Applications: A Combined Experimental & Computational Study

Abstract: Metal-organic frameworks (MOFs) are a class of porous materials characterized by their tunable structures and high porosity, which make them suitable for a wide range of applications, including gas storage, separation, catalysis, and drug delivery. Among them, MOF-5 and UiO-66 are worth mentioning because of their easy synthesis, low production cost, or water stability. Despite being prototypes, a few notable limitations make them unsuitable for some specific applications. For example, we cannot use MOF-5 for semiconductor or visible light absorption applications. Its water stability is also not remarkable. Likewise, despite being stable, UiO-66's luminescence and catalytic properties are not very prominent. Our study integrates computational modeling and experimental techniques to address these key issues and broaden their application domains. Computational methods, such as density functional theory (DFT), with different experimental techniques (PL, PXRD, IR, SEM, BET, TGA) are used to predict selected MOFs' structural stability, sensing behavior, adsorption properties, etc. Our studies consider these well-recognized MOFs with suitable modification strategies, such as doping, post-synthetic modification (PSM), or ligand replacements.

References:

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- Biswal, D. P.; Singha, D., Panda, J.; Rana, M. K. “Post-Synthetic Modification of Zr-based Metal-Organic Frameworks with Imidazole: Variable Optical Behavior and Sensing”, *ChemPhysChem* **2023**, 24, *e20230031*.

Bio sketch :

Dr. Malay Kumar Rana is currently an Assistant Professor at the Department of Chemical Sciences at IISER Berhampur, India. He received his Ph.D. degree from the Department of Chemistry, IIT Kanpur, India, under the supervision of Prof. Amalendu Chandra in 2010. Afterward, he did postdoctoral work at the Department of Chemistry & Pharmacy, University of Sassari, Italy (2010-2011), and the Department of Mechanical Engineering, University of Michigan, USA (2011-2015). Prior to joining IISER Berhampur in 2016, he also worked as a senior scientific officer at the National Centre for Flexible Electronics at IIT Kanpur, India. His current research focuses on the development of effective therapeutics for COVID-19, cancer, and bacterial infections, including studies on porous, crystalline nanomaterials and 2D materials for optoelectronics, sensing, gas separation and energy storage applications. State-of-the-art computational methods and complementary experiments are used in his research.

T24: Prof. Basudev Sahoo

Affiliation: IISER THIRUVANANTHAPURAM

Title: Photocatalytic C-C Bond Functionalization of Ketone-Derived Dihydroquinazolinones

Abstract: Ketone functionality is highly ubiquitous in natural products, (pre)clinical drugs, and commodity chemicals.[1] Compared to vastly explored nucleophilic addition to C=O bond and □ C-H functionalization, recently, the evolution of catalytic C-C bond functionalization of aliphatic ketones remains sought-after for streamlining organic synthesis.[2] Unstrained (di)ketone-derived pro-aromatic compounds serve as alkyl/acyl radical precursors via aromaticity-driven C-C cleavage enabled by photocatalysis or metal catalysis.[2-4] Among other precursors, dihydroquinazolinones have recently received considerable momentum as adaptative C(sp^3) synthon in catalytic C-C bond functionalization, including our contributions to various C-C and C-X bond forming transformations (Figure 1).[3,4]

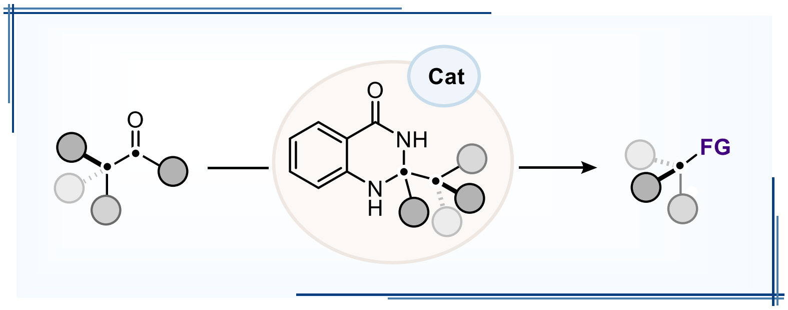

Figure 1: C-C bond functionalization of unstrained ketones via dihydroquinazolinones

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Bio sketch :

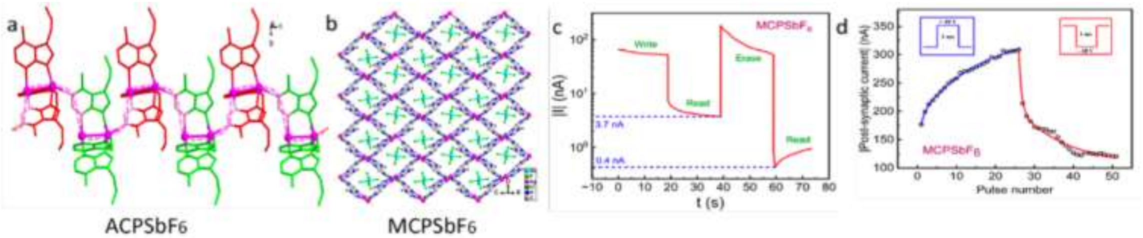
Dr. Basudev Sahoo completed his BSc in chemistry from the Ramakrishna Mission Residential College, affiliated to the University of Calcutta in 2009 and MSc in Chemistry from the Indian Institute of Technology (IIT) Kanpur in 2011. Then, he moved to Germany to pursue his PhD under the supervision of Prof. Frank Glorius at the University of Muenster. After completing his PhD in 2015, he moved to the group of Prof. Matthias Beller at the Leibniz Institute for Catalysis (LIKAT), Rostock, Germany as a Leibniz Postdoctoral Fellow. In 2018, he received Marie Curie (MSCA) postdoctoral fellowship and joined the group of Prof. Ruben Martin at the Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain. Currently, he is an associate professor in the school of chemistry, IISER Thiruvananthapuram. He was one of the recipients of Thieme Chemistry Journals Award 2022. His group is pursuing research on organic synthesis and catalysis enabled by transition metal catalysis and visible photocatalysis.

T25: Prof. Chandra Shekhar Purohit

Affiliation: NISER BHUBANEHSWAR

Title: Homo-Dimetalic Silver Purine Complexes as Neuromorphic Materials

Abstract: Various materials explored for bioinspired neuromorphic devices like afferent nerves,1 optoelectronic sensors, 2 olfactory neurons,3 adaptive biosensors,4 and optomemristors.5 We synthesized few MOFs with 7-methylchloropurone and 7-allylchloropurine (Scheme -1) that gives di-metallic silver-purine complexes having Ag-Ag bonds. These materials are showing interesting electrical conductivity, and are studied for neuromorphic computing such as LTP, LTD, and STDP. A Six-terminal neuromorphic device with MCPSbF6 complex shows heterosynaptic neural computing with an endurance of 2800 cycles and a retention time exceeding 6 hours.

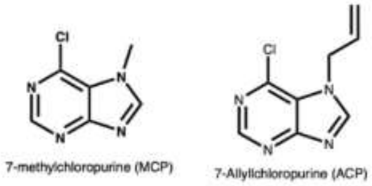


ACPSbF6

MCPSbF6

Figure 1 (a) Crystal structure of ACPSbF6 (b) Crystal structure of MCPSbF6 (c) retention time in the device made with MCPSbF6 in LRS state after writing and reading (d) Postsynaptic current vs. pulse number showing LTP, LTD.

Scheme-1:



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Bio Sketch:

Associate Professor, NISER, Bhubaneswar (Since, 2019); Joined NISER in 2010.

PhD: IIT Kanpur (2003-2008)

Post doc: AvH fellow at LIMES, University of Bonn, Germany (2008-2009)

Research publication: 70 publications in National / International journals.

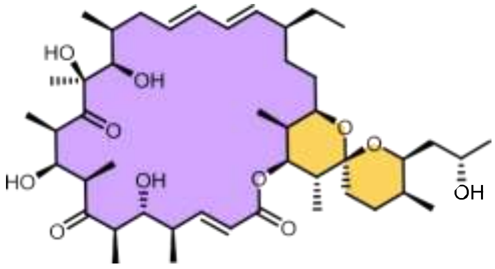
Research area: Bio-organic chemistry and Supra-molecular assemblies

T26: Prof. Rajesh V

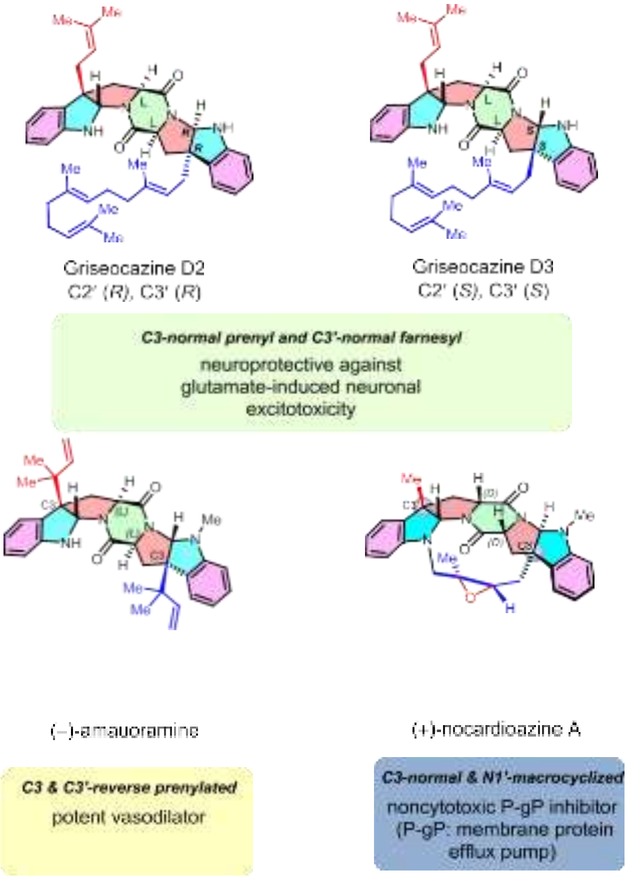
Affiliation: IISER TIRUPATI

Title: Biomimetic Pathways towards Therapeutic Natural Products

Abstract: Natural products form a significant portion of therapeutics that improve human health. Historically, the field of natural products have garnered tremendous excitement from various perspectives. My research group looks at Natural Products mechanistically: from marine *Nocardiopsis to indigenous tribal plant species native to India*, we harness Nature's biosynthetic machinery.



Oligomycin A
$C_{45}H_{74}O_{11}$
$[M+Na]^+$ m/z:813.5089



Our recent publications reveal the diverse range of problems we have tackled, from biomimetic chemistry to discovery of biocatalysts. In this seminar, we highlight biomimetic syntheses of neuroprotective Griseocazines and the discovery of spiroketal-containing Type- I polyketide antibiotics from *Trichopus zeylanicus* (an indian medicinal plant).

References:

Nature Communications, **2023**, *14*, 2558; *J. Org. Chem.*, **2022,** *87,* 11519-11533; *ACS Omega*, **2021,** *6*,

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30, e202401782; DOI: https://doi.org/10.26434/chemrxiv-2025-v596v; *J. Biosci.* **2021,** *46*:37; *J. Med. Chem.* **2018,** *61*, 666-680; *Proc. Natl. Acad. Sci. U. S. A.,* **2017,** *114,* 8241-8246.

Bio sketch:

Rajesh Viswanathan received his master's degree in Chemistry from Indian Institute of Technology, Kanpur in 1999. His MS-thesis project was on peptidomimetics with Prof. Javed Iqbal. His Ph. D. studies were in synthetic organic chemistry from Indiana Univ. in 2005 under the supervision of Prof. Jeffrey N. Johnston. His thesis work focused on strategies for total synthesis of cyanobacterial alkaloids. He was a postdoctoral fellow with Prof. Dale Poulter at the University of Utah, USA, where he developed prenyltransferase-based chemoenzymatic strategies to construct biosensors. Subsequently, he joined Case Western Reserve University (Dept. of Chemistry) as an Assistant Professor. He was promoted to Frank Hovorka Assistant Professor and received Faculty Excellence Award (2014) and was the Gamma Sigma Alpha Outstanding Prof. awardee in 2016. He was the student invited speaker at the NIH-RISE program seminars held at the University of Puerto Rico (San Piedras Campus) in 2016. At Case Western, he served as the Board member for the Small Molecule Drug Discovery Core [SMDDC] and a Co-Investigator for a Program Project Grant, funded by the National Institutes of Aging (NIH P01). He serves as a consultant chemist for Gingko Bioworks, Boston – a synthetic biology firm interested in sustainable platforms for production of fine chemicals and perfumes.

He joined Indian Institute of Science Education and Research (IISER), Tirupati in 2018 and currently a Professor and the Dean, Academics. His research program has received SERB-CRG award (Organic Chemistry) and the National Science Foundation grant (NSF-CHE-award). His lab's research advances in the area of biocatalysis has led to a start-up, Avian Biovolatiles, as a joint venture between IISER and IIT Tirupati, where he holds the CSO position. He serves as an Editorial Board member of the *Journal of Biosciences* (Springer and IASc). His research groups' interests are broadly in the areas of organic synthesis, natural product biosynthesis and the design and development of enzyme inhibitors as anticancer agents.

T27: Prof. Jeetender Chugh

Affiliation: IISER PUNE

Title: Probing conformational heterogeneity in an RNA recognition motif: implications for fibril formation

Abstract: Fused in Sarcoma (FUS), a protein implicated in neurodegenerative diseases contains N- and C-terminal LC-rich regions, a zinc finger motif flanked by two RG-rich regions, and a single RNA-recognition motif (RRM). While FUS-RRM is highly soluble and exists as a monomer in solution, upon agitation, it undergoes amyloid-like aggregation. Since the fibrils and the fibril formation pathways are implicated in neurodegenerative diseases, it is of utmost importance, from a drug discovery point of view, to find detailed molecular insights into the fibrillation process. Here, we investigated the conformational heterogeneity of FUS-RRM using NMR relaxation-dispersion experiments. We observed that the monomer (M) exists in a dynamic exchange with multiple excited states (ES), which gets quenched to varying extents by altering the protein environment. The perturbation of ES is then shown to have implications in the type of fibrils formed. The data suggests a coupling of the conformational heterogeneity to aggregation kinetics wherein ES probably acts as a switch that controls the fibrillation process under pathophysiological conditions. These results add to the understanding of the fibrillation process, thereby paving the way for a better understanding of the role of FUS in neurodegenerative diseases.

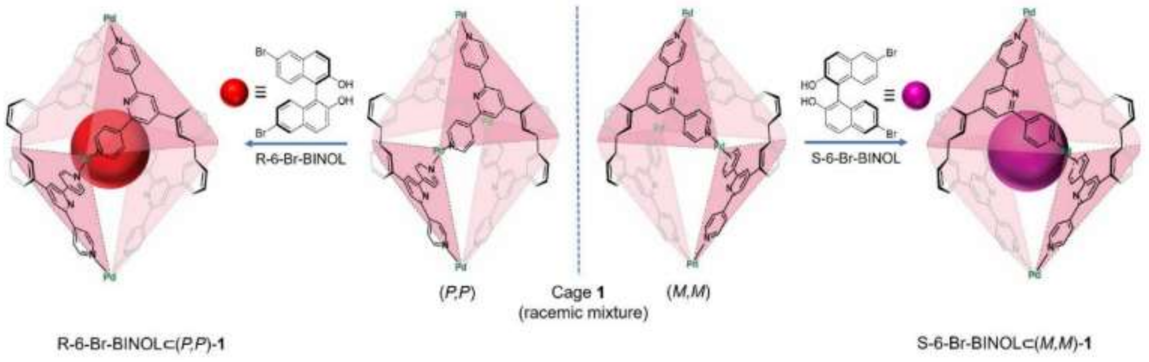
Bio sketch:

T28: Prof. Dipak Samanta

Affiliation: NISER BHUBANESWAR

Title: **Self-Assembled Coordination Cages: Exploring Chiral Induction and Iodine Capture**

Abstract: Self-assembled coordination cages represent a versatile platform for addressing complex challenges in molecular recognition and environmental remediation. This talk will focus on recent advances in the design and functionalization of palladium-based coordination cages, exploring their novel applications in two distinct areas: chiral induction and environmental capture of iodine. The precise control of chirality at the molecular level remains a key challenge in chemistry, particularly in the context of enantioselective catalysis and asymmetric synthesis. In this study, we developed a Pd4-based self-assembled cage that is achiral by design. However, upon the introduction of chiral guest molecules, we observed the transfer of chirality from the guests to the cage itself. This process of chiral induction is driven by specific host-guest interactions, leading to the formation of chiral cage complexes. We will discuss the underlying mechanisms, the influence of different guest molecules on the chiral induction process, and the potential applications of these systems in areas such as enantioselective catalysis, chiral separation, and sensing technologies. This work opens new pathways for designing responsive and adaptable molecular systems capable of fine-tuning their chiral properties based on environmental inputs. In a parallel study, we designed nonporous amorphous coordination cages with N-heteroatom functionality, enabling the efficient capture and storage of iodine. This system addresses a critical need for environmental solutions in radioactive iodine management, offering a scalable and selective approach to sequestration. Together, these innovations showcase the flexibility and power of coordination cage chemistry in both molecular recognition and environmental applications.



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4. R. Singha, P. Maity, D. Samanta, Chem. Eur. J. 2024, e202401013

5. P. Maity, H. Pradhan, A. Das, M. Dalapati, D. Samanta, Chem. Eur. J. 2024,

e202400328.

Bio sketch:

Dr. Dipak Samanta is an Assistant Professor at the National Institute of Science Education and Research (NISER) Bhubaneswar, specializing in supramolecular chemistry and coordination-driven self-assembly. His research focuses on the design and synthesis of metal-organic architectures for applications in molecular recognition, separation processes, and stimuli-responsive materials. Dr. Samanta earned his Ph.D. in Chemistry from IISc Bangalore, where he developed expertise in the construction of self-assembled coordination cages. His postdoctoral work further honed his skills in dynamic molecular systems and host-guest chemistry. At NISER, Dr. Samanta leads a research group dedicated to exploring the potential of coordination cages in various applications, including selective molecular encapsulation and environmental remediation. His notable publications include studies on reversible photoswitching of encapsulated azobenzenes in water, and the development of flexible coordination cages exhibiting reversible chromism. Dr. Samanta's contributions to the field have been recognized through various awards and honors. He is committed to advancing the understanding of supramolecular systems and mentoring the next generation of chemists.

T29: Prof. Somrita Ray

Affiliation: IISER BERHAMPUR

Title: **Enhancing the rate of a gated drift-diffusion process by optimal restart**

Abstract: “Gating” is a popular terminology in biochemistry that narrates the transition between the activated (or open) and deactivated (or closed) states of an ion-channel that makes transport through the channel highly selective. In general, gating is a mechanism that imposes an additional restriction on a transport, as the process ends only when the “gate” is open and continues otherwise. When diffusion occurs in the presence of a constant bias to a gated target, i.e., to a target that switches between an open and a closed state, the transport essentially slows down compared to the corresponding ungated drift-diffusion process, resulting in an increase in the mean completion time. In this work [1], we utilize stochastic restart as an external protocol to counterbalance the delay due to gating. In particular, we consider a particle that undergoes drift-diffusion in the presence of a stochastically gated target and is moreover subjected to rate-limiting resetting dynamics. Calculating the minimal mean completion time rendered by an optimal resetting rate for this exactly solvable system, we construct a phase diagram that owns three distinct phases: **(i)** where resetting can make gated drift-diffusion faster even compared to the original ungated process, **(ii)** where resetting still expedites gated drift-diffusion but not beyond the original ungated process, and **(iii)** where resetting fails to expedite gated drift-diffusion. Gated drift-diffusion aptly models various stochastic processes such as chemical reactions that exclusively take place in certain activated states of the reactants. Our work predicts the conditions under which stochastic restart can act as a useful protocol to enhance the rate of such processes without compromising on their selectivity.

Reference:

[1] A. Biswas, A. Pal, D. Mondal, and **S. Ray***, *J. Chem. Phys.* **159**, 054111 (2023).

Keywords: Stochastic processes; drift-diffusion; mean first-passage time; stochastic resetting; gating.

Bio sketch:

Present Position (since Jan. 2024) :

• Assistant Professor, Department of Chemical Sciences, IISER Berhampur, India.

Post-doctoral Research Experience :

• **Dec. 2022 − Jan. 2024:** Elizabeth Gardner Fellow*, School of Physics & Astronomy, University of Edinburgh, UK [*independent research position for 4 years].

• **Jan. 2021 − Nov. 2022:** DST-INSPIRE Faculty Fellow, Department of Chemistry, IIT Tirupati, India [**on-lien** from Dec. 2022 − Jan. 2024].

• **Jun. 2018 − Dec. 2020:** Distinguished Postdoctoral Fellow, School of Chemistry, Tel Aviv University, Israel [**Advisor: Dr. Shlomi Reuveni**].

• **Mar. 2016 − Jun. 2018:** Postdoctoral Guest Scientist, Division Biological Physics, MPIPKS, Dresden, Germany [**Advisor: Dr. Andre C. Barato**].

Education :

• **Ph.D** in **Chemistry**, Visva-Bharati University, India in 2015 [**Advisor** : **Dr. Bidhan Chandra Bag**]. • **M.Sc.** in **Chemistry**, University of Calcutta, India in 2010 (First Class, **Rank 2**). • **B.Sc.** in **Chemistry** (Hons.), Presidency College, University of Calcutta, India in 2008 (First Class).

Awards/Recognition/Fellowships received :

• Awarded **Elizabeth Gardner Fellowship** by the School of Physics & Astronomy, University of Edinburgh, UK in May, 2022 (for a 4-year independent research position).

• Received **INSPIRE Faculty Award** in Chemical Sciences by DST, India in April, 2020. • Received **Outstanding Reviewer Award** for *Journal of Physics A: Mathematical and Theoretical* in 2019 by the **Institute of Physics (IOP)**, London.

• Awarded **Sackler Postdoctoral Fellowship** by the Raymond and Beverly Sackler Center for Computational Molecular and Materials Science, Tel-Aviv University, Israel. • Awarded Scholarship for **Short-Term Visit** to MPIPKS, Dresden, Germany in 2022 and 2025. • Qualified **NET Examination** in Chemical Sciences as CSIR-JRF in 2010 and awarded Doctoral Research Fellowship by CSIR, India (August, 2010 − August, 2015).

T30: Prof. Sudipta Roy

Affiliation: IISER TIRUPATI

Title:

Biosketch:

T31: Prof. Soumit Mondal

Affiliation: IISER TIRUPATI

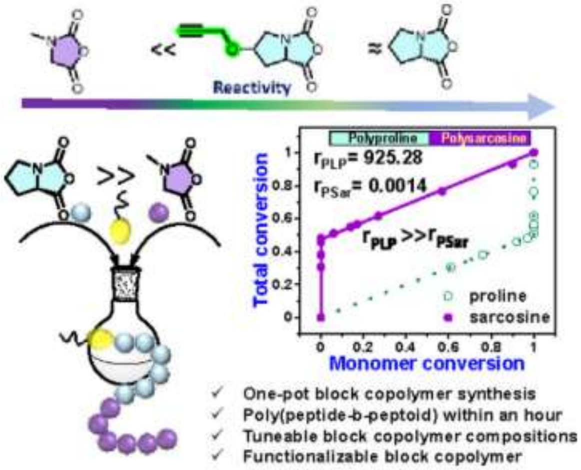
Title:

Biosketch:

T32: Prof. Raj Kumar Roy

Affiliation: IISER MOHALI

Title: **A kinetically regulated methodology for the synthesis of sequence-controlled polypeptides**



Abstract: The three-dimensional structure of proteins is essential for their biological functions, determined by the sequence of monomers that dictate their spatial orientation and interactions. In contrast, synthetic copolymers are random distributions of at least two different monomers. Researchers have sought to bridge the gap in structural control between biomacromolecules and synthetic polymers.[1] Block copolymers can be efficiently prepared using controlled or living polymerization, which involves sequential addition of monomers but is often labor-intensive. Single-step synthesis methods, such as one-pot sequential polymerization, switchable polymerization, orthogonal chemistry, and kinetically controlled processes, show promise for efficient block copolymer creation. Kinetically controlled processes are particularly noteworthy for their flexibility in defining copolymer structures, including alternating and gradient forms, relying on reactivity ratios from the kinetics of homopolymerization and copolymerization.

Recently, Lu and colleagues showcased the water-assisted ring-opening polymerization (ROP) of proline-NCA monomers.[2] Unlike previously established polymerization methods, this innovative approach promotes a homogeneous ROP of polyproline. It dramatically speeds up the polymerization process, reducing the time required from several days to just a few minutes. While exploring the water-assisted ring-opening polymerization of sarcosine NCA monomers, we observed that the kinetics were notably slower than those of proline-NCA monomers. This observation prompted us to investigate the potential for sequence-controlled ring-opening copolymerization of both proline and sarcosine-NCA monomers. In my presentation, I will outline the one-pot poly(peptide-b-peptoid) synthesis achieved through the ring-opening copolymerization of selected pairs of N-carboxy anhydride (NCA) monomers.[3] Furthermore, I will demonstrate the synthesis of complex polypeptide structures through this kinetically controlled approach

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3. Maity, P.; Bisht, A. S.; Deepak.; Roy, R. K. *ACS Macro Lett*. **2025**, *14*, 188.

Bio sketch:

Dr. Raj Kumar Roy received his MS (2008) and Ph.D. degree (2012) from IISc Bangalore in polymer chemistry under the supervision of Professor S Ramakrishnan. His doctoral research focused on synthetic polymer chemistry, particularly hyperbranched polymers, and their functionalizations. He did postdoctoral research (2012-2015) in Strasbourg, working on sequence-controlled and sequence-defined polymers synthesis under the supervision of Professor Jean-Francois Lutz, and subsequently moved to Nagoya University, Japan, as a VBL research fellow and JSPS postdoctoral fellow (2015- 2017) and worked in the area of helical polymers under the supervision of Professor Eiji Yashima. He joined IISER Mohali in 2017 as an Assistant professor. His current research focused on precision polymer synthesis, functionalized polypeptides, organic multiferroic materials, and foldamers.

T33: Prof. Pritam Mondal

Affiliation: IISER MOHALI

Title: Mimicking Met-Tyr-Trp Crosslink Cofactor Biogenesis in Catalase-peroxidase KatG using Synthetic Porphyrin Iron(III) π-dication Species

Abstract: The heme-containing enzymes catalase-peroxidases (KatG), which possess both peroxidase and catalase activities, post-translationally incorporate a unique cofactor with two covalent cross-links formed between tryptophan (Trp), tyrosine (Tyr), and methionine (Met) residues on the distal side of the catalytic heme center.[1,2]In prokaryotic KatG, it has been demonstrated that this peculiar Met-Tyr-Trp adduct, in its entirety, is fully essential for the catalase activity and that its presence has a strong influence on the electronic structure and spectroscopic signatures of the redox intermediates of KatG.[2] Although there are many documented cases of heme enzymes possessing amino acid-amino acid or amino acid-heme cross-links in Nature, precise mechanistic details pertaining to such cross-link formation are largely unknown till date.[1,3] Few proposals have advanced to account the involvement of either a heme-compound-I or - hydroperoxo active species in the formation of Met-Tyr-Trp adduct, however, definitive experimental evidence is nonexistent for or against either of those proposed pathways. To elucidate the mechanistic pathway of such cross-link cofactor biogenesis, herein we model the Met-Tyr-Trp crosslinking using diphenyl sulfide, indoles and substituted phenols as methionine, tryptophan and tyrosine analogue, respectively and octa-fluorinated iron (III) porphyrin [$\mathrm{Fe^{III}}$F8TPP] as heme mimic. Highly reactive heme-dication [$\mathrm{Fe^{III}}$F8TPP^{++}]$^{+}$intermediate[4](an isoelectronic species to high-valent Compound-I) was generated cryogenically, and its reactivity towards a series of indoles and substituted phenols have been performed, which showed a facile conversion into their corresponding cross-coupled products. Similarly, diphenyl sulfide immediately reacts with indole phenol coupled species in presence of heme-dication intermediate and forms the Met-Tyr-Trp mimic. A fully substantiated mechanistic proposal has been put forward, which closely resembles several key attributes proposed in the analogous KatG enzyme shedding important light on the cross-coupling mechanism.

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2. Ghiladi, R. A.; Knudsen, G. M.; Medzihradszky, K. F.; De Montellano, P. R. O. *J. Biol. Chem.* **2005**, *280*, 22651-22663.

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Bio sketch:

Dr. Pritam Mondal obtained his Ph.D. in 2017 in the field of inorganic supramolecular chemistry under the guidance of Prof. S. P. Rath in the Department of Chemistry at the Indian Institute of Technology, Kanpur. Then he moved to the laboratory of Prof. Gayan B. Wijeratne in the Department of Chemistry, University of Alabama at Birmingham, USA, where he worked on synthetic heme enzymes and their reactivity landscapes. He joined the Department of Chemical Sciences at IISER Mohali in August 2023, and his research interest lies in elucidating mechanistic details of heme/non-heme enzymes through biomimetic modelling.

T34: Prof. Sachin Dev Verma

Affiliation: IISER BHOPAL

Title: In-situ Visualization of Nanostructure Growth using Interferometric Scattering (iSCAT) Microscopy

Abstract: Understanding the growth mechanism of metal nanostructures, such as silver and gold nanorods, is crucial due to their diverse applications in fields like biomedicine, electronics, imaging, and environmental science.[1] Insights into their growth mechanisms are crucial, as they enable control over the size, shape, and morphology of nanorods, allowing for the customization of these structures for specific applications.[2]

To investigate growth mechanisms, we have developed interferometric scattering microscopy,[3] enabling direct in-situ observation of nanostructure growth in real-time. This non-invasive, label-free technique allows for the observation of kinetics in the seed-mediated growth[4] of silver, and gold nanorods. The growth begins with seed nanoparticles acting as nucleation points for metal ion reduction and deposition. Observations reveal that, in case of silver, the growth process is not a straightforward transition from spherical seeds to elongated rods; instead, seeds grow into relatively larger structures that may disintegrate into fragments, which subsequently reassemble to form the final nanorods. Understanding the intermediate steps of such complex growth behaviour is crucial for optimizing the synthesis and applications of metal nanorods.

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(3) Young, G.; Kukura, P. Interferometric Scattering Microscopy. *Annu. Rev. Phys. Chem.* **2019**, *70* (1).

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Bio sketch:

Academic Qualifications:

PhD	*Jawaharlal Nehru University*	2013

Professional Experience:

Post-doc	*University of South Carolina*, Columbia South Carolina, USA	2013-2016
	University of California, Irvine California, USA	2016-2017
	University of Cambridge, Cambridge Cambridgeshire, UK	2017-2019
Assistant Professor	IISER Bhopal	2019-present

Awards & Achievements:

- *CRSI Young Scientist Award* (2025), by the Chemical Research Society of India
- *2023 Rising Star in Measurement Science*, by ACS Meas. Sci. Au
- *Member, Early Career Advisory Board*, Chemical Physics Impact (Elsevier)
- *Marie Skłodowska-Curie Fellow* (2017-2019)

About Yourself:

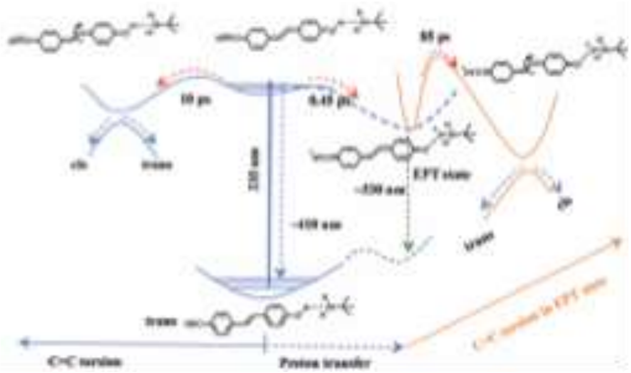
Dr. Sachin Dev Verma is an Assistant Professor at IISER Bhopal, where he has been contributing to the academic and research community since 2019. His group explores ultrafast carrier dynamics in semiconductor nanostructures, excited-state processes in organic semiconductors. His group has developed an advanced technique to analyse relaxation rate-dispersion, two-dimensional fluctuation correlation spectroscopy (2D-FlucCS), that focuses on differentiating heterogeneous and homogeneous systems using 2D correlation analysis. Recently, his group has developed interferometric scattering (iSCAT) microscopy to understand the early-stage dynamics, and intermediate steps involved in nanostructure growth.

T35: Prof. Adithya Lakshmanna

Affiliation: IISER THIRUVANANTHAPURAM

Title: Ultrafast Structural Dynamics in Molecular Adducts Featuring Photo-initiated Proton-coupled Electron Transfer

Abstract: The capture and control of early-time events of molecules and materials upon photoexcitation lies at the heart of ultrafast spectroscopy. Unraveling the excited state dynamics that are typically governed by a complex interplay of various factors such as substituents, intramolecular and intermolecular interactions pose serious challenges to traditional linear spectroscopic techniques. In this talk, I shall demonstrate that a judicious mix of diverse ultrafast nonlinear spectroscopic techniques such as femtosecond transient absorption spectroscopy, fluorescence upconversion, and stimulated Raman spectroscopy can lead to deciphering the intricacies in complex excited state dynamics. I shall describe the ultrafast excited-state structural dynamics in molecular adducts involving photoacids and photobases such as 4-cyano-4'-hydroxystilbene:*tert*-Butylamine, 4-dimethylamino-styrylpyridine:hexafluoroisopropanol, 4-Hydroxychalcones:*tert*-Butylamine, and provide an analysis of the spectroscopic signatures associated with the photo-initiated proton-coupled electron transfer reactions in these systems.



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Verma, P.; Mitra, P. K.; Adithya Lakshmanna, Y. (2025, Communicated).

Bio sketch:

Y. Adithya Lakshmanna obtained an integrated B. Sc. Ed degree from Regional Institute of Education, Mysore and an M. Sc. Degree in Physics from Indian Institute of Technology, Madras. Subsequently, he pursued PhD in Physical Chemistry from Indian Institute of Science, Bangalore working under the supervision of Prof. S. Umapathy. Adithya is currently an assistant professor at the School of Chemistry, Indian Institute of Science Education and Research Thiruvananthapuram. His research interests are broadly in the direction of addressing the excited-state reaction dynamics that are mediated by fundamental processes such as electron transfer, proton transfer, and proton-coupled electron transfer. His research group employs a multitude of time-resolved spectroscopic techniques that include time-resolved Raman, infra-red, and circular dichroism spectroscopy.

T36: Prof. A. Muthukrishnan

Affiliation: IISER THIRUVANANTHAPURAM

Title: Metal-Free Oxygen Electrocatalysts: Defects vs Heteroatom(s)

Abstract: Metal-free heteroatom-doped carbon nanomaterials are promising alternatives to high-cost state-of-the-art platinum catalysts and less stable second-generation non-platinum group metal oxygen reduction/evolution reaction (ORR/OER) catalysts. Understanding the origin of the active sites in the heteroatom-doped carbon material plays a vital role in designing novel electrocatalysts for ORR/OER in energy storage and conversion systems. Various active sites such as defects (edge and topological), heteroatoms (doped with higher or lower electronegative non-metals), heteroatoms-induced, cooperative (synergistic) effect (two different heteroatoms, defect-heteroatom) can be the potential active sites. In this presentation, we try to evaluate the contributions of individual active sites towards oxygen reduction. The improvements in the ORR activity from the defect-only carbon materials to a heteroatom(s)-doped materials were studied to understand the real active sites of the metal-free heteroatom(s)-doped carbon electrocatalysts.

Bio sketch:

Dr.A.Muthukrishnan joined as an assistant professor in the school of chemistry, Indian Institute of Science and Education Research Thiruvananthapuram, in June 2017. He received his M.Sc degree from the Indian Institute of Technology Madras, and later, he joined the same department and received his PhD in July 2010. Later, He worked as a post-doctoral researcher at Prof. Takeo Ohsaka's group, Tokyo Institute of Technology, Japan, on developing active and durable carbon alloy catalysts for fuel cell cathodes. The work includes identifying active sites of non-platinum group metal nitrogen-doped carbon catalysts by exploring the oxygen reduction reaction mechanism. In January 2017, he joined as an assistant professor at the School of Chemistry, University of Hyderabad. After a short period in Hyderabad, he became an assistant professor at IISER Thiruvananthapuram. Currently, he is working in the area of designing non-platinum group metal and metal-free fuel cell electrocatalysts to understand the active site information using fundamental concepts and developing new materials using the kinetic and mechanistic insights.

T37: Prof. Moumita Majumdar

Affiliation: IISER PUNE

Title: Orbital engineering of heavier group 14 and 15 cationic compounds for catalytic functions

Abstract: We are interested in tuning the frontier electronics of the heavier Group 14 and 15 elements in their regular or low-oxidation states and develop new catalytic manifolds by translating their unique electronic features into creative catalysts.[1],[2] Along this direction in Group 14 chemistry, we have established the intramolecular donor stabilized tetra-coordinated Ge(IV) di-cations as Lewis acid catalysts in recent times.[3] Therein, we have reported the preliminary tests on the catalytic hydrosilylation of benzaldehyde using the Ge(IV) di-cations as catalysts. Further investigations reveal that the choice of the donor groups manipulate the extent of Lewis acidity at the Ge centre and thus serve as versatile catalysts for various organic transformations. We have studied element-element cooperative reactivity using heavier Group 15 elements.[4] The cationic distibane and dibismuthane compounds synthesized can activate small molecules. The concepts developed in our group in terms of modulating the geometry and electronics of these positively charged compounds for catalytic applications will be discussed.

Keywords: catalysis, main-group elements, cations

References:

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Bio sketch:

Moumita Majumdar obtained her PhD for research on Transition-Metal Multiply Bonded Systems from Indian Institute of Technology, Kanpur, India in 2010. Subsequently, she joined as Assistant Professor (specially appointed) in the group of Prof. Kazushi Mashima, Osaka University, Japan, where she worked on Metal Cluster Catalysis. In 2011, she moved to Germany for second post-doctoral stint in the group of Prof. David Scheschkewitz, Saarland University, where she gained expertise in Low-Valent Silicon Chemistry. Her current research interests are Low-Valent Main Group Compounds in catalysis and materials applications.

Research Interests:

Research in Dr. Moumita Majumdar's group is focused on expanding the chemical functionalities of low-valent compounds spanning the Groups 13-15 of the periodic table. Arguably, the heavier main-group elements have fundamentally different electronic properties from their lighter congeners, which have always intrigued the molecular chemists. The ongoing research in the group is much directed in their syntheses and state-of-the-art applications. Among the major research targets are: (1) Designing intricate main-group ligands such as (poly)cationic donor ligands that effortlessly binds to transition metals for their implications in Lewis acid catalysis; (2) Cooperative interactions on a main-group platform; (3) Main-group and Transition metal cluster chemistry; (4) Photo-luminescent properties of main-group compounds; (5) Organometallic approach to designing main-group materials for energy-related applications.

Awards and Honors

1 Recipient Chemical Research Society of India (CRSI) Bronze Medal in 2024

2 Selected in She Is - 75 Women in Chemistry by the Royal Society of Chemistry and The Office of the Principal Scientific Adviser to the Government of India, 2023

3 Recipient of Alexander von Humboldt Fellowship for experienced researchers 2022

4 Recipient of SERB-POWER Fellowship 2022

5 *Chem. Comm*. Emerging Investigator 2020

Positions Held

1 Editorial Advisory Board Member, *Inorganic Chemistry*, American Chemical Society, 2023-2025

2 International Advisory Board Member, *Chem. Asian J.* Wiley-VCH, from 2022

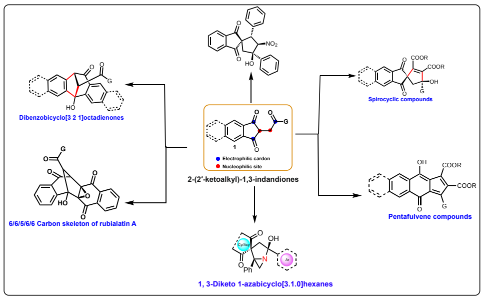
3 Early Career Advisory Board Member, *ChemistryOpen*, Wiley-VCH, from 2022

T38: Prof. Thirupathi Barla

Affiliation: IISER BERHAMPUR

Title: 2-Keto-1,3- Indandione, a Versatile Ingredient for the Synthesis of Medicinally Important Carbocyclic- and Heterocyclic-Compounds

Abstract: 2-keto-1,3-indandiones serve as an important precursor for the construction of various bicyclic, spiro cyclic systems with suitable partners. Accordingly, the reaction of arynes with 2-keto-1,3-indandiones provided dibenzobicyclo[3.2.1]octadienone core[1] and the reaction of dimethyl acetylene dicarboxylate (DMAD) with 2/3-keto-1,3-Indandiones afforded spiro[4.4]nonane, spiro[4.5]decane compounds in the presence of a catalytic amount of DABCO.[2] Moreover, the spiro[4.4]nonanes were transformed into highly conjugated pentafulvene motifs via unprecedented C-C bond rearrangement in an acidic medium. Similarly, we have also developed a catalyst-free method to access various 1,3-indandione-containing spiropyrrolines.[3] Additionally, we have achieved the synthesis of complex, multiring, spirocyclic, 1,3-dicarbonyl fused, and highly functionalized 5-phenyl-1-azabicyclo[3.1.0]hexanes (ABCH) from 2-keto-1,3-indandiones.[4]



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Bio sketch:

Dr. Thirupathi Barla was born in Madavelli, Manchirial district, Telangana, India 1984. After completing his M.Sc. (Organic Chemistry) from Osmania University (2006-2008), he worked as a research chemist at Aragen Life Sciences, formerly known as GVK-Biosciences, Hyderabad (2008-2009). In early 2009, he joined as a Junior Research Fellow (JRF) at CSIR-Indian Institute of Chemical Technology, Hyderabad, with Dr. D. K. Mohapatra for doctoral studies (2009-2014). Afterwards, he worked as an associate research scientist in the process R&D division at Sai Life Sciences, Hyderabad (2014-2015). Then Dr. Barla moved to Harvard University as a postdoctoral fellow to work with Prof. E. J. Corey (2015-2018), where he was involved in the development of highly active fluorinated second-generation oxazaborolidine catalysts and their application in Diels-Alder reactions. In July 2018, he joined as an assistant professor of Chemistry at the Indian Institute of Science Education and Research Berhampur. Subsequently, he is promoted to Associate Professor in February 2024. Dr. He is a recipient of the Thieme Chemistry Journal Award **2023**. Thirupathi's area of research includes developing novel carbon-corban bond formation reactions and their application towards natural product synthesis. Dr. Thirupathi's group is also working on the total synthesis of biologically active natural products or model compounds having potential bioactivities.

T39: Prof. Parikshit Moitra

Affiliation: IISER BERHAMPUR

Title: Development of Novel Nanomaterials for Molecular Diagnosis of Certain Clinical Manifestations

Abstract: We are developing new nanomaterials and conjugating them with suitably tuned complementary oligonucleotides. These oligonucleotides are chosen based on their target binding energy and binding site disruption energy with their target sequence. The oligonucleotide-conjugated nanomaterials were characterized by various analytical techniques including UV-visible spectroscopy, fluorescence spectroscopy, X-ray diffraction, Raman spectroscopy, scanning electron and transmission electron microscopy. These nanomaterials are then used for molecular diagnosis of various clinical manifestations. Changes in spectroscopic data were recorded to selectively detect the presence of targeted genetic material. In this talk, I shall be presenting two such cases recently being developed in my laboratory.

Keywords: Covalent Organic Framework; Gold nanoparticles; Complementary Oligonucleotides; Clinical Diagnosis.

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3. Neethu K M et al, Use of Quantum Dots as Nanotheranostic Agents: Emerging Applications in Rare Genetic Diseases, Small 2025, DOI: https://doi.org/10.1002/smll.202407353

Biosketch:

EDUCATION

Doctor of Philosophy (Ph.D.), Bio-organic Chemistry, 2010-2015 Indian Institute of Science, Bangalore, Karnataka, India

(Thesis submitted on 29th July, 2015, defended on 6th April 2016;

Degree awarded on 25th June 2016)

Thesis Advisor – **Professor Santanu Bhattacharya**

“Title of PhD thesis: Syntheses and Characterization of Novel Materials for Efficacious Anticancer Drug Delivery and Selective Sensing of Bioanalytes”

Master of Science (M. Sc.) in Chemical Sciences, 2008-2010 Indian Institute of Science, Bangalore, Karnataka, India

(Degree awarded on 25th June 2016)

Bachelor of Science (B. Sc.) with Honours in Chemistry, 2005-2008 Rahara Ramakrishna Mission Vivekananda Centenary College,

University of Calcutta, Kolkata, West Bengal, India

EMPLOYMENT HISTORY

Assistant Professor, Jan 15, 2024 – Present Department of Chemical Sciences,

IISER Berhampur,

Berhampur, Odisha, India

Assistant Research Professor, July 5, 2022 – Jan 12, 2024 Department of Nuclear Engineering,

The Pennsylvania State University,

University Park, Pennsylvania 16802, United States

With Professor Dipanjan Pan

Research Associate, Dec 7, 2020 – July 4, 2022 Department of Pediatrics, Center of Blood Oxygen Transport and Hemostasis,

University of Maryland Baltimore School of Medicine,

Baltimore, Maryland 21201, United States

With Professor Dipanjan Pan

Postdoctoral Associate, Nov 25, 2019 – Dec 6, 2020 Department of Pediatrics, Center of Blood Oxygen Transport and Hemostasis,

University of Maryland Baltimore School of Medicine,

Baltimore, Maryland 21201, United States

With Professor Dipanjan Pan

Scientist D, Feb 21, 2017 – Nov 22, 2019 Technical Research Centre,

School of Applied and Interdisciplinary Sciences (SAIS),

Indian Association for the Cultivation of Science (IACS),

Poster Presentation Abstracts

Title: Electrostatically driven unidirectional molecular flux for high performance alkaline flow batteries

Student Name: BHOJKUMAR NAYAK

Affiliation: IISER PUNE

Poster Code: P-01

Abstract: To address the discrepancy between energy supply and demand caused by diurnal and seasonal fluctuations, significant efforts focus on storing renewable energy using diverse energy storage technologies. Redox flow batteries are advantageous over traditional types due to their ability to separate energy and power functions. However, critical interfacial processes like mass transport and electron transfer profoundly influence the energy storage and conversion mechanisms of flow batteries. We demonstrate that activation of electrostatic forces at interfaces enables directional molecular flux to and from electrode surfaces, generating concurrent or counteracting electrostatic and diffusion currents. This strategy enhances flow battery volumetric energy density and increases energy efficiency up to approximately 92%, while preserving the redox active species' solubility limit.

Title: H-Bond Directed Non-Covalent Dimer Formation & Supramolecular Polymerization of a Chiral Naphthalene Diimide (NDI) System

Student Name: SAYANTAN KHAN

Affiliation: IISER KOLKATA

Poster Code: 02

Abstract: Supramolecular polymerization of π-conjugated systems has gained significant attention due to its relevance in optoelectronics, chiral sensing, and biomimetic assemblies. Herein, we present a hydrogen1bond (H-bond) directed self-assembly of a chiral Naphthalene Diimide (NDI) system, where non-covalent interactions (NCIs) govern the formation of well-defined supramolecular architectures. The system undergoes aggregate-to-aggregate transformation over time, revealing pathway complexity in supramolecular organization. By strategically incorporating chiral tail substituents at the NDI core, we investigate the reaction dynamics of supramolecular polymerization, focusing on the thermodynamic and kinetic aspects. Time1dependent circular dichroism (CD) spectroscopy is employed to track the kinetic evolution of chiral aggregates, showing that the saturation time of θ values at a fixed wavelength increases with increasing concentration. This suggests a competitive pathway mechanism (A → M → B), where A represents the kinetically controlled aggregate, M the monomeric state, and B the thermodynamically stable aggregate. Variable-temperature UV-Vis and NMR spectroscopy further elucidate the formation of non-covalent dimers as primary assembling units, which subsequently elongate into hierarchical supramolecular structures. Our findings highlight the role of H-bonding motifs in directing self-assembly, where competing nucleation-growth and isodesmic models dictate structural evolution. The observed aggregate-to1aggregate transformation with increasing time and concentration-dependent pathway competition emphasize the dynamic adaptability of these supramolecular systems. These insights provide a deeper understanding of pathway complexity and morphological transitions, paving the way for designing responsive molecular materials with tunable properties. Keywords: Chirality, Pathway complexity, Self-assembly, Naphthalene diimide (NDI), H-bonding References – 1. P. A. Korevaar, S. J. George, A. J. Markvoort, M. M. J. Smulders, P. A. J. Hilbers, A. P. H. J. Schenning, T. F. A. de Greef, E. W. Meijer, Nature 2012, 481, 492 – 496 2. J. Matern, Y. Dorca, L. Sánchez, G. Fernández, Angew. Chem. Int. Ed. 2019, 58, 16730 – 16740 3. M. Wehner, M. I. S. Röhr, M. Bühler, V. Stepanenko, W. Wagner, F. Würthner, J. Am. Chem. Soc. 2019, 141, 6092 − 6107 4. M. A. Jinks, M. Howard, F. Rizzi, S. M. Goldup, A. D. Burnett, and A. J. Wilson, J. Am. Chem. Soc. 2022, 144, 23127 − 23133

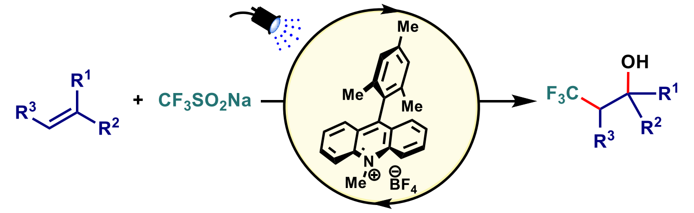
Title: β-Hydroxytrifluoromethylation of Unactivated Alkenes via Visible Light Mediated Organophotoredox Catalysis

Student Name: MOUSUMI BEHERA

Affiliation: IISER PUNE

Poster Code: 03

Abstract: Trifluoromethylation is a pivotal transformation in organic synthesis.[1] Introduction of a trifluoromethyl group significantly enhances the electronegativity, lipophilicity, and metabolic stability of molecules. As a result, trifluoromethylated compounds have found widespread applications in pharmaceuticals, agrochemicals, and advanced materials. While the hydroxytrifluoromethylation of activated alkenes, such as styrenes, has been achieved using transition metal catalysis, the direct functionalization of unactivated alkenes remains challenging due to their inherent inertness and high oxidation potential. Recent breakthroughs in visible light photoredox catalysis have provided an eco-friendly and efficient alternative for such transformations. Although metallaphotocatalysts have shown promise, their reliance on transition metal catalysts limits sustainability. Remarkably, no reports exist on organophotoredox-catalyzed β-hydroxytrifluoromethylation of unactivated alkenes. Addressing this gap, we present a transition metal-free strategy employing an organophotoredox catalyst under visible light, enabling a mild, efficient, and sustainable approach to accessing β-trifluoromethylated alcohols at room temperature.[2] This work paves the way for greener and more versatile synthetic methodologies.[3]



♦Transition metal-free ♦Terminal & internal alkenes ♦Diverse functional group tolerance
♦Functionalization of natural products ♦Feasible under sunlight ♦Scalable up to 0.5 g

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2) **Behera**, **M.**; Dharpure, P. D.; Sahu, A. K.; Bhat, R. G. *J. Org. Chem.* **2024***, 89,* 14695–14709.

3) **Behera**, **M.**; Shukla, S. Y.; Dharpure, P. D.; Bhat, R. G. *ChemRxiv* **2024**, DOI: 10.26434/chemrxiv-2025-p2cbf

Title: Deciphering the Bonding in Metavalent Materials for Next-Generation Memory

Student Name: DR. GAURAV JHAA

Affiliation: IISER MOHALI

Poster Code: 04

Abstract : Phase change materials have garnered significant attention due to their applications in phase change memory (PCM) technology, which can surpass the Von Neumann bottleneck via in-memory computing. This is particularly useful in artificial intelligence applications requiring rapid data transfer. Therefore, identifying the bonding mechanism in such materials is crucial as it will aid in designing better materials for PCM applications. In this context, a new bonding mechanism named metavalency, indicating a chemical bond between metallic and covalent, was introduced recently to describe the bonding in phase change materials. The metavalent materials are characterized by nearly half bond order, large Born Effective Charge (BEC), low band gap, moderate electrical conductivity, and large optical dielectric constant. However, their bonding features overlap significantly with the well-known hypervalent and partial bond systems, raising fundamental questions about whether metavalency constitutes a truly distinct bonding mechanism. Here, we employ molecular orbital theory and DFT calculations to identify the unique bonding in known metavalent materials and compare them with hypervalent half-bond order systems that are not classified as metavalent. We show that the metavalent compounds are characterized by partial σ bonds formed mainly by p-p overlap and have low ionicity. Crucially, we demonstrate that if such systems have low band gaps either due to low bonding-antibonding splitting or due to delocalization, that results in large BEC. This refined understanding of metavalent bonding provides a foundational framework for the rational design of novel PCMs, paving the way for

advancements in phase-change memory technology. REFERENCES 1. Wuttig, M.; Yamada, N., Phase-change materials for rewriteable data storage. Nature Mater 2007, 6 (11), 824-832. 2. Sevison, G. A.; Farzinazar, S.; Burrow, J. A.; Perez, C.; Kwon, H.; Lee, J.; Asheghi, M.; Goodson, K. E.; Sarangan, A.; Hendrickson, J. R.; Agha, I., Phase Change Dynamics and TwoDimensional 4-Bit Memory in Ge2Sb2Te5 via Telecom-Band Encoding. ACS Photonics 2020, 7 (2), 480-487. 3. Sebastian, A.; Le Gallo, M.; Eleftheriou, E., Computational phase-change memory: beyond von Neumann computing. J. Phys. D: Appl. Phys. 2019, 52 (44), 443002. 4. Wuttig, M.; Deringer, V. L.; Gonze, X.; Bichara, C.; Raty, J.-Y., Incipient Metals: Functional Materials with a Unique Bonding Mechanism. Adv. Mater. 2018, 30 (51), 1803777 5. Jhaa, G.; Kumari, M.; Chakkingal Parambil P.; In pursuit of understanding metavalency. ChemRxiv. 2025; doi:10.26434/chemrxiv-2025-8856v-v2

Title: Colour Removal of Binary Mixture of Food Coloring Dye by Fenton Oxidation: Effect of Water Matrix, E330, and Kinetics

Student Name: Dr. JOHN ELISA

Affiliation: IISER PUNE

Poster Code: 05

Abstract: Food coloring dyes, such as Food Red 9 (FR9) and Food Green 3 (FR3) which are widely used in the food industry, this dyes due to their intense colour when released to water streams without treatment, disturb the photosynthetic activity and decrease the soil quality and affect the plant growth which increase the level of danger to aquatic animals. To address these issues, the present study investigates the color removal of a mixture of two food coloring dyes (FR9 + FG3) using Fenton oxidation and optimizes its parameters using a face-centered central composite design. The optimum parameters are found to be $[\mathrm{FR9} + \mathrm{FG3}]_0$ = 0.34 mM; $[\mathrm{Fe}^{2+}]$ = 0.3 mM; $[\mathrm{H_2O_2}]$ = 4.0 mM at pH 3.0; agitation = 200 rpm; Temp = 25°C. A colour removal efficiency of 47.78 and 93.45 % was found after 120 min of treatment at 422 and 624 nm, respectively. The effect of different water matrix parameters was studied, and it was observed that the presence of nitrate ions increases the removal efficiency, while other inorganic anions inhibit it. The colour removal efficiency of Fenton increased by 3.9 and 3.1 fold for 422 nm and 624 nm, respectively, after adding E330. Different kinetic models like zero- first- second-order and BMG kinetic models were employed, and the best fit was found to be the BMG kinetic model.

Title: Reduction of Nitrite at First-row Late Transition Metals: Insights into the Role of Metals

Student Name: ADARSH CK

Affiliation: IISER TVM

Poster Code: 06

Abstract: The reduction of nitrite (NO_2^-) is an important biochemical process due to its significance in biogeochemistry and physiology.[1] For example, nitrite anion serve as a source of nitric oxide (NO) under hypoxia in mammalian physiology. Copper and iron sites of various metalloenzymes are well known to catalyze nitrite to NO.[2] Recently, it was found that redox inactive zinc containing carbonic anhydrase enzyme could convert nitrite to NO via HNO_2 intermediate.[3] These examples demonstrate that the reduction of nitrite follows distinct mechanistic pathways, depending on the metal present at the active site. Model complexes have been widely employed to understand the underlying mechanisms involved in these biological processes. It is noteworthy that the interaction of biological redox cofactors such as thiols and phenols with the metal center is crucial for the activation of nitrite at the metal centers.

We herein employ a series of mononuclear metal(II)-nitrite complexes, and their reactivity towards various reducing agents such as phenols, thiols, and acids were studied. Interestingly, we observed that the redox and the lewis acidity of the metal center plays a pivotal role in the nitrite activation. A detailed study provides insights into the underlying mechanism and the factors controlling the NO generation from nitrite at different metal(II) sites.

Reference

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Title: A nonheme mononuclear iron(II) chloride complex and its oxygen atom transfer (OAT) reactivityStudent

Name: Soumojyati Prodhan

Affiliation: IISER PUNE

Poster Code: 07

Abstract: The Fe^{II}/2-oxoglutarate-dependent (Fe/2OG) halogenases are a class of Fe/2OG enzymes that can hydroxylate or halogenate unactivated C-H bond for the purpose of biosynthesis of different organic molecules.[1,2] These Fe/2OG enzymes have two histidine units and 2-oxo-

glatarate unit in its active site.[3] The key intermediate generated by these halogenases is a chloroferryl intermediate, which can favour halogenation over hydroxylation by modification of the substrate binding cavity.[4,5,6] In this project we have synthesized a nonheme mononuclear iron(II)chloride complex that shows different reactivity towards dioxygen and PhIO. The μ-oxo-diiron(III)dichloro complex which is generated upon reaction with PhIO in absence of substrates suggests the formation of a chloroferryl intermediate, which demonstrates oxygen atom transfer (OAT) reactions in presence of substrates.

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Title: Molecular Packing Induced Long Living Trap States in Oligothiophene based Self-assembled Nanoparticles for Photocatalytic Solar Hydrogen Production

Name: Soham Ghosh

Affiliation: IISER BERHAMPUR

Poster Code: 08

Abstract: Two different types of self-assembled nanomaterials have been fabricated from 2,2'-Bithiophene-5,5'-dicarboxaldehyde (BTDA) and 2,2':5',2"-Terthiophene-5,5"-dicarboxaldehyde (TTDA) molecules through solvent assisted reprecipitation methods. During self-assembly formation, TTDA molecules become randomized through partial face-to-face interactions, resulting in the formation of defect mediated emissive trap state at longer wavelength region The emissive trap states are charge-transfer types and also possess longer decay times compared to pristine molecules. It is further supported by computational and femtosecond transient absorption spectroscopy studies. The appearance of the trap state due to random molecular packing in TTDA nanoparticles further facilitates the free electron accumulation, which helps to boost the photocatalytic solar H_2 production. However, the development of a defect-mediated emissive trap state was inhibited by the highly defined head-to-tail molecular arrangements of BTDA molecules during self-assembly formation. The photocatalytic efficiency of BTDA nanoparticles therefore decreases. Our findings point to the critical role that defect-mediated emissive trap states play in photocatalysis, which will pave the way for the advancement of small molecule-based self-assembly as a novel class of molecular materials for solar energy conversions.

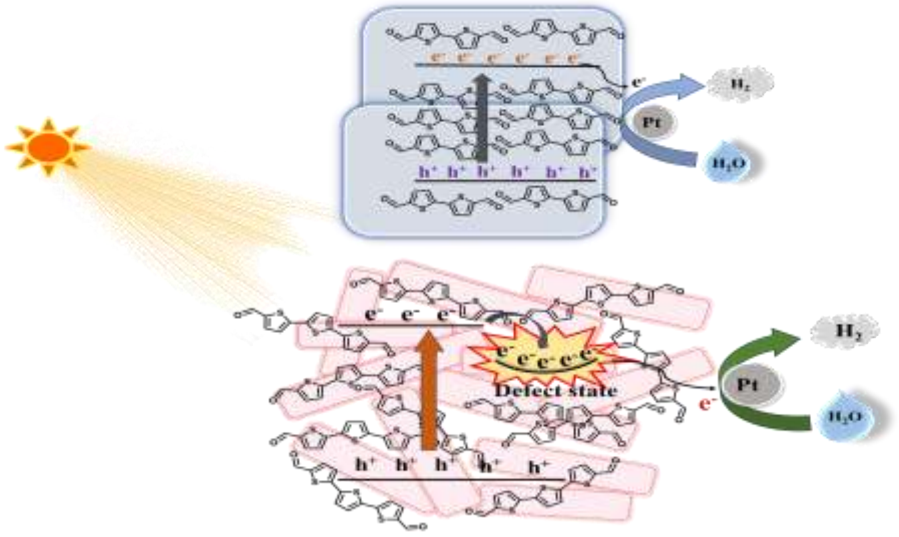

Figure 1: Mechanism for photocatalytic hydrogen production from self-assembled organic nanoparticles.

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Title: Engineering Steric Effect for Efficient Thermally Activated Delayed Fluorescence with Non-linear Optical Properties

Name: Madhusudan Dutta

Affiliation: IISER PUNE

Poster Code: 09

Abstract: Multi-carbazole-based benzonitrile systems are efficient thermally activated delayed fluorescence (TADF) materials for organic light-emitting diodes (OLEDs). However, they suffer from low PLQY due to large dihedral angle arising from steric crowding. Addressing this challenge, in this work we demonstrate a potent strategy to engineer steric crowding. To achieve our goal, we have designed three novel emitters, namely, CzPHCN, tCzPHCN and Cz2CzPHCN based on phenanthrene-9,10-dicarbonitrile (PHCN), as an acceptor core to minimize the steric hindrance between the donor groups. Among the three molecules, tCzPHCN exhibits a maximum PLQY of 86% and the highest RISC rate of 11.6×10^5 s^{-1}, the underlying cause being the least dihedral angle of 45.72° and suppressed intermolecular interaction due to the presence of bulky

tert-butyl group. Unlocking a new realm of application, the unique non-centrosymmetric space group (*$Cmc2_1$*) of CzPHCN offers excellent SHG with $\chi^{(2)}$ value of 0.21 pm V^{-1} at 1320 nm with laser-induced damage threshold (LIDT) value of 37.82 GW cm^{-2}.

Title: Integrating Ensemble Machine Learning and MD Simulations for Discovering NNRTIs against HIV-1 Reverse Transcriptase

Name: Anvesha Shree

Affiliation: IISER BERHAMPUR

Poster Code: 10

Abstract: The Human Immunodeficiency Virus (HIV) has been a global challenge since long and necessitates a continuous discovery of novel therapeutic agents to improve the efficacy of currently available options and overcome resistance. This study presents an accelerated and cost-efficient machine-learning-based ensemble approach to identify the potential non-nucleoside reverse transcriptase inhibitors (NNRTIs) against the HIV-1 Reverse Transcriptase (HIV-1 RT) enzyme. A stacking ensemble model is developed, combining predictions from various base models. Using a ChEMBL-derived dataset of experimentally tested compounds against HIV-1 RT, the model achieved 90.30% accuracy and 89.43% ROC-AUC, and was then deployed on the Natural Product Atlas (NPA) database to predict active molecules. The molecules were evaluated for their physicochemical and ADMET properties, docked into the allosteric pocket of the RT heterodimer, and selected complexes were subjected to 1 μs molecular dynamics (MD) simulations to assess their stability. Among these, the compound designated as NP1 demonstrated the greatest stability within the NNRTI binding pocket and showed superior efficacy than Doravirine (DOR) in inhibiting RT dimer activity. Furthermore, a potential metapath was identified from the polymerase site to the RNase H site of p66 via the NNIBP, involving the residues of p51, which may play a crucial role in the global allosteric regulation of the complex. We propose NP1 as a lead compound, characterized through a combination of stacking ML model and MD simulation, exhibiting robust stability and superior inhibitory potential against HIV-1 RT.

Title: Hole Doping of S = ½ Kagome Antiferromagnet CoCu3(OH)6Cl2

Name: Rimpa Mandal

Affiliation: IISER PUNE

Poster Code: 11

Abstract: Geometrically frustrated magnetic materials with spin ½, known as Kagome lattice, a two-dimensional corner sharing triangular lattice, have been explored for topological and correlated electronic and magnetic phenomena. These Kagome lattices are typically electrical insulators. Hence, doping such systems with electrons/holes could bring the fascinating transformation of an insulator to a semiconducting or metallic system. Herein, we have adopted an unconventional strategy of doping an S = ½ Kagome lattice $CoCu_3(OH)_6Cl_2$ (CuCo-H), a structural analog of a well-known quantum spin liquid (QSL) candidate herbertsmithite ($ZnCu_3(OH)_6Cl_2$), by integrating it with reduced graphene oxide (rGO) via in situ redox chemistry. In the course of the reaction, GO (graphene oxide) was reduced to rGO, and simultaneously, Cu(I) ions were oxidized to Cu(II) ions. The substitution of Zn by Co in the interlayer of herbertsmithite leads to the strong exchange of antiferromagnetic coupling along with hole doping in the Kagome from the rGO matrix. Estimated magnetic moments, Hall-effect measurements, Bader charge analysis, and photoemission signals together provide the signature of hole doping in the Kagome. As a result of the hole doping, the electrical conductance value was remarkably enhanced from $\sim10^{-11}\ \Omega^{-1}$ (CuCo-H) to $\sim10^{-4}\ \Omega^{-1}$ (CuCo-H-rGO) while retaining the magnetic frustration. Such spin-frustrated Kagome semiconductors can potentially behave as quantum materials and may find interesting applications in memory devices, superconductors, and quantum computing.

References:

1. K. Gupta et al., ***J. Phys. Chem. Lett.*** 2019, 10, 2663-2668
2. R. Mandal et al., ***Adv. Phys. Res.*** 2024, 2400037

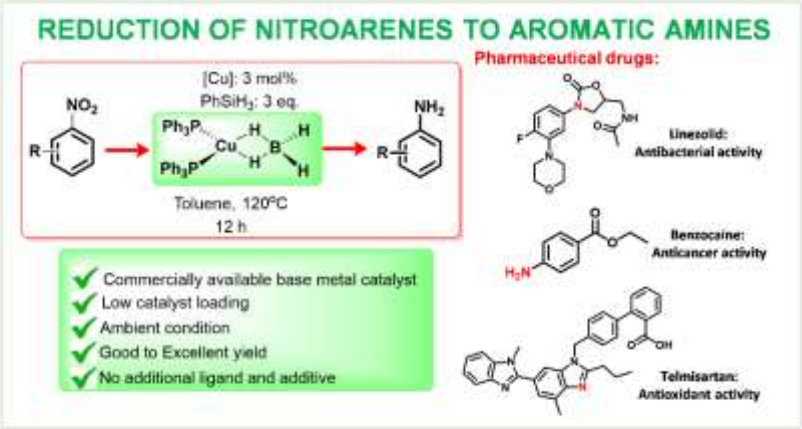
Title: Copper Catalyzed Hydrosilylation of Nitroarenes: Chemoselective Reduction to Aromatic Amines

Name: Pritirekha Mallick

Affiliation: NISER BHUBANESHWAR

Poster Code: 12

Abstract: Reduction of nitroarenes to aniline derivatives is an important transformation in synthetic organic chemistry as well as in industry. In this context, hydrosilylation is considered as an easier alternative as compared to well-established Béchamp reduction[1] and classical hydrogenation.[2] Various noble metal based catalytic hydrosilylation protocols were developed for the nitroarene reduction.[3] However, the number of reports using base metals as catalyst for the same purpose is limited.[4] No reports have been published on copper-catalyzed hydrosilylation of nitroarenes. In fact, copper is considered as one of the most ignored base metals in various hydrofunctionalization reactions, including hydrosilylation. Hence, development of a copper catalyzed hydrosilylation protocol for the reduction of nitroarene is important. In this regard, an efficient catalytic hydrosilylation protocol was developed for the reduction of nitroarenes to aromatic amines by utilizing a commercially available copper(I) complex. Various nitroarenes with diverse functional groups were effectively reduced. Very good chemoselectivity was observed in the presence of other reducible functionalities. The practical utility of this copper catalyzed hydrosilylation of nitroarene was further demonstrated through the syntheses of various drug molecules and pharmaceutical intermediates.



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Title Tailoring Potential Ferroelectric Properties in Conformationally Switchable Er(III)-Isothiocyanates Using Organic Cation Modulation

Name: RISHUKUMAR PANDAY

Affiliation: IISER PUNE

Poster Code: 13

Hybrid molecular ferroelectrics, due to their facile synthesis and robust physical properties, have emerged as a new class of functional materials. Such systems require flexible parts that can lock into two different positions and thereby switch the polarity of the crystal in a reversing electric field. Isocyanate ligands display this kind of behavior in their usual non-linear coordination. Using triethyl methyl ammonium (**TEMA**) cations yields the salt **$[TEMA]_4[Er(NCS)_7]$** that shows a phase transition denoted by the Aizu notation *mmm*F*mm*2 at 203 K. In contrast, the bulkier phosphonium cation ethyltriphenyl phosphonium (**ETPP**) yielded the high-T_c (or effectively T_c-free) ferroelectric **$[ETPP]_3[Er(NCS)_6]$**. The polarization vs. electric field (*P*-*E*) loop measurements on a single crystal gave a saturation polarization (P_s) of 1.43 μC cm^{-2}, while dielectric measurements revealed the absence of a paraelectric phase (T_c) close to the melting point (483 K). It also exhibits the piezoelectric charge coefficient (d_{33}) of 22.7 pC N^{-1}. Finally, thermoplastic polyurethane composite devices of **$[ETPP]_3[Er(NCS)_6]$** were investigated for mechanical energy harvesting applications.

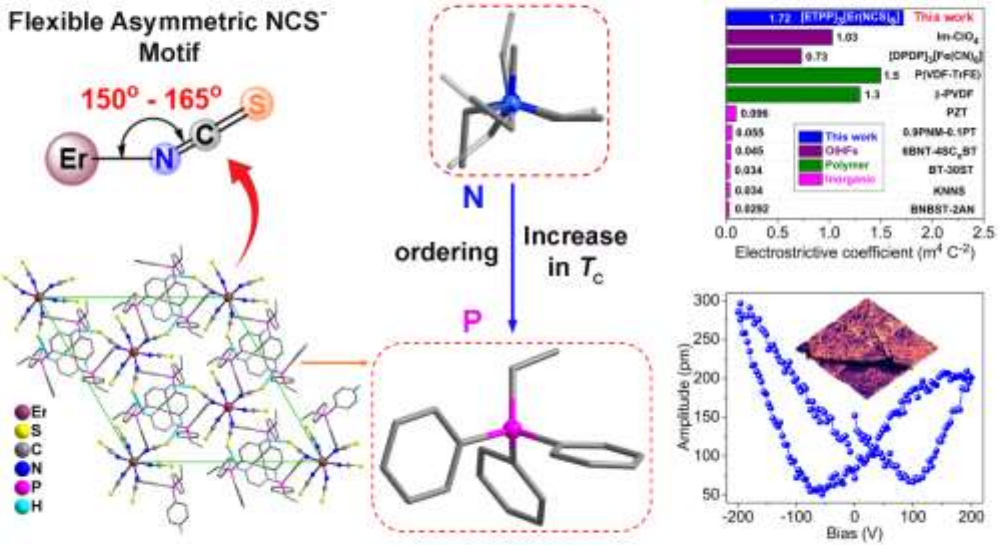

Figure 1 Designing strategy of molecular ferroelectrics and its high piezoresponse behavior from conformationally switchable Er(III)-NCS motif.

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Title: **Red-Light Driven Supramolecular Photocatalysis: Functionalization of Photoinert N-Propargyl amides to Substituted oxazole**

Name: SATHI SAHOO

Affiliation: NISER BHUBANESWAR

Poster Code: 14

Abstract: energy source for environmentally friendly chemical transformations. However, its broader use is limited by a scarcity of catalysts effective under mild conditions and diverse light spectra, requiring innovative strategies beyond traditional designs. Supramolecular photocatalysis exemplifies such innovation, utilizing dynamic, self-assembled complexes to explore novel reaction pathways. This study introduces an approach involving photo-inert *N*-propargyl benzamides, which are assembled *via* chelation into a second-order inner metallic complex in the presence of KO^{t}Bu. These systems (λ_{em} = 502 nm, τ = 0.96 ns) harnessed visible red light (620–750 nm) to trigger a self-sustaining catalytic cycle. Upon red light absorption by the complex, a single-electron transfer (SET) occurred from the counter anion to its building block, facilitating the solvent-free synthesis of 2,5-disubstituted oxazoles with 100% atom economy. This small molecule reaction system effectively could mimic the function of a photosynthetic reaction center within the system**.**

Figure: A chelation-assisted self-assembled supramolecular photocatalysis, triggering the functionalization of 2-*halo*-propargyl amides under neat conditions.

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Title: Superstructures of Copper Nanoclusters as NIR TADF Emitters: Solvent-dependent Optical-Morphological Modulation and Catalytic Activity

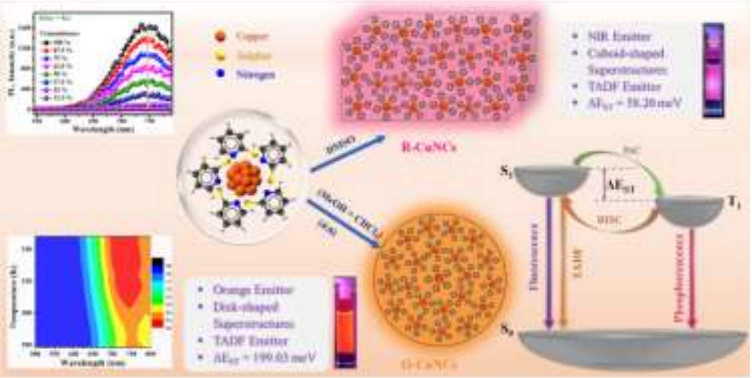
Name: SAMEEKSHA AGRAWAL

Affiliation: IISER BHOPAL

Poster Code: 15

Abstract. Luminescent materials that emit in the near-infrared (NIR) range, have garnered tremendous attention in the fields of chemistry, biomedical, and material science due to several advantages over conventional fluorophores, including less scattering, and greater stability. Herein, we report 2-

mercaptopyridine-templated copper nanoclusters (CuNCs) with NIR emission in both solid and colloidal states. The emission can be shifted to orange by using a methanol-chloroform mixture instead of water. This change in photophysical properties correlates with morphological tuning. The strong NIR emission arises from thermally activated delayed fluorescence (TADF), confirmed by long excited state lifetime, Time Resolved Emission Spectroscopy (TRES) measurements, temperature-dependent photoluminescence studies, temperature-dependent lifetime studies, and excitation-transmittance dependent TRES intensity measurements. CuNCs exhibit a small singlet-triplet energy gap (58.2 meV), indicating efficient TADF. The solvent-dependent morphological tuning of the nanocluster superstructures rendering drastic change in the photo-physical signatures is the consequence of different $\Delta E_{(S1\text{-}T1)}$ values for the CuNCs in different solvent environments.



Scheme 1: *Schematic representation of the morphological variation of the superstructures of CuNCs in two different solvent environments and their respective properties.*

Further findings corroborate that the electronic structure of the surface ligands can also help us to tune the $\Delta E_{(S1\text{-}T1)}$ energy gap for these nanoclusters. Moreover, by smart molecular imprinting of the surface ligands we can achieve the formation of water soluble NIR-TADF emitting nanoclusters with exceptional catalytic activity in a representative redox reaction.

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Title: Ultrafast Charge Carrier Dynamics of All-inorganic 2D Ruddlesden-Popper Phase Perovskite Nanocrystals

Name: IPSITA PARCHHA

Affiliation: NISER BHUBANESWAR

Poster Code: 16

Abstract: All inorganic Ruddlesden-Popper (RP) phase perovskite materials have gained remarkable attention for their unique optical properties and extreme thermal stability. Elemental doping in these materials can provide an effective approach to further modify the structural, optical and magnetic properties. However, the fundamental understanding of the ultrafast photophysical processes and the effect of doping in these materials has never been explored and, hence, needs a comprehensive investigation. In this study, we have synthesized Mn-doped RP phase perovskite Cs2PbI2Cl2 nanoplatelets by using the hot injection method and investigated the comprehensive charge carrier dynamics employing Photoluminescence (PL), time-resolved PL and femtosecond transient absorption (TA) spectroscopy. The TA study demonstrates a faster depopulation of high-energy states with a minimal alteration in the band edge kinetics upon doping in the system. This clearly suggests the hot electron transfer from the host Cs2PbI2Cl2 to the Mn2+ states dominated over band edge electron transfer, which is further supported by the time-resolved PL measurement. These findings provide new insight into the hot carrier dynamics in RP phase perovskites and can be advantageous for designing hot carrier-based efficient photovoltaic devices.

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Title: **Visible Light-Induced Sequential Nitrogen Insertion and Benzotriazolation of Quinoxaline-2(1H)-ones**

Name: SHANKHAJIT MONDAL

Affiliation: IISER PUNE

Poster Code: 17

Abstract: A visible light-mediated sequential reaction involving in situ generation of benzotriazole from benzene-1,2-diamine and *tert*-butyl nitrite and further concomitant cross-coupling with quinoxaline-2(1*H*)-ones via C–N bond formation in one pot will be described in the poster. The developed protocol uses metal-free mild conditions and demonstrates 36 examples of ≤80% yield with wide functional group tolerance.

Title: **N-Fused and Non-fused Carbapentaphyrins: A Strategy for Controlling Fusion**

Name: Adrija Kayal
Affiliation: NISER BHUBANESHWAR

Poster Code: 18

Abstract: Pentaphyrins are a class of expanded porphyrins consisting of five pyrrole rings connected by five meso-carbon bridges. 1 The integration of arene units in the macrocyclic core results in the formation of carba-pentaphyrins. Flexibility of such macrocycles arises due to an increase in core size, and often offers accessibility towards ring-inversion significantly. This can substantially affect their reactivity in several cases by facilitating or reinforcing, fusion reactions inside the core. The formation of fusion in the core also modifies the π-circulation pathways, which can consequently alter the macrocycle's aromatic properties. In 2008, Osuka and coworkers reported the synthesis of N-fused pentaphyrin with Möbius aromaticity. 2 Earlier studies demonstrated the formation of N-fused and non-fused pentaphyrins depending on the quantity of the oxidizing agents used and also documented the generation of meso-free non-fused pentaphyrins as a result. 3 Diverse examples have shown that the nature of substituents at the meso-positions can promote distortion of the macrocyclic structure.4 However, reports of meso substituents dictating the regulation of N-fused and non-fused products are rare. Herein, we wish to report the synthesis of N-fused and non-fused poly-phenyl embedded macrocycle, by controlling the steric bulk at the meso-position, and demonstrated their aromatic characteristics.

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Title: Nano-Springe Enriched Hierarchical Porous MOP/COF Hybrid Aerogel: Efficient Recovery of Gold from Electronic Waste

Name: Dipanjan Majumder

Affiliation: IISER PUNE

Poster Code: 19

Abstract: Extraction of gold from secondary resources such as electronic waste (e-waste) has become crucial in recent times to compensate for the gradual scarcity of the noble metal in natural mines. However, designing and synthesizing a suitable material for highly efficient gold recovery is still a great challenge. Herein, we have strategically designed rapid fabrication of an ionic crystalline hybrid aerogel by covalent threading of an amino-functionalized metal-organic polyhedra with an imine-linked chemically stable covalent organic framework at ambient condition. The hierarchically porous ultralight aerogel featuring imine-rich backbone, high surface area, and cationic sites have shown fast removal, high uptake capacity (2349 mg/g), and excellent selectivity towards gold sequestration. Besides, the aerogel can extract ultra-trace gold-ions from different terrestrial water bodies, aiming towards safe drinking water. This study demonstrates the

great potential of the composite materials based on a novel approach to designing a hybrid porous material for efficient gold recovery from complex water matrices.

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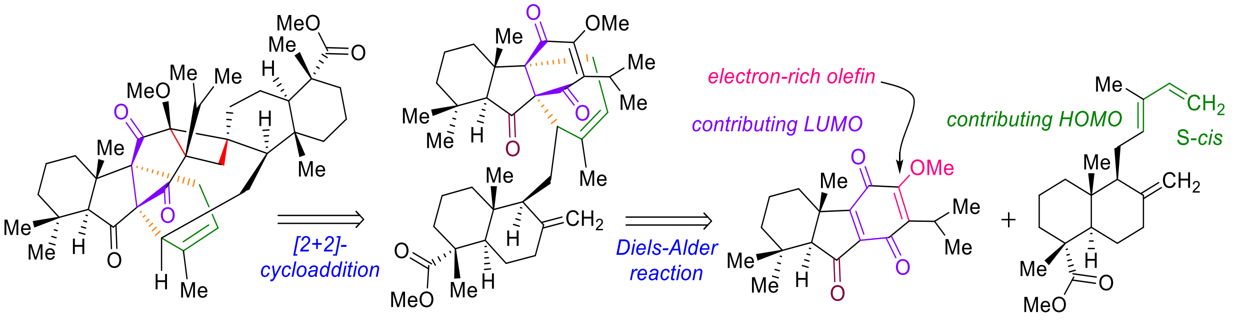
Title: **Asymmetric Total Synthesis of Naturally Occurring Tetraterpenoid, Taiwaniadduct J**

Name: Suman Noskar

Affiliation: IISER KOLKATA

Poster Code: 20

Abstract: The first enantioselective total syntheses of taiwaniadducts I, J, and L, complex tetraterpenoids with promising biological activity are accomplished through an only 23-step longest linear sequence, demonstrating excellent regioselectivity, guided by steric and electronic factors. In 1997, biogenesis-inspired chemical research of the leaves of *Taiwania cryptomerioides* by Fang *et. al.* afforded the most complex molecule of taiwaniadduct class of tetraterpenoids, taiwaniadduct J.[1] The nortetraperpenoid features dense oxidative functionalities in a tetracyclic heptodecane core which arises from *abeo*-abietane scaffold (6/5/6-fused ring system) where a *p*-benzoquinone core showed Diels-Alder reactivity with a labdane diterpenoid. As well, the molecular complexity also arises due to photoinduced [2 + 2]-cycloaddition reaction resulting into cyclobutane motif with contiguous quaternary stereocenters.[1]



taiwaniadduct J bismethylated taiwaniadduct I *abeo*-abietane core *trans*-ozic acid methyl ester

Figure-1. Structures and retrosynthetic precursors of Taiwaniadduct J.

Our hypothesis to craft this potentially bioactive tetraterpenoid is via pericyclic reactions, drawing inspiration from Mother Nature's potential biogenesis. Also, the literature study reveals that the biosynthesis of both abietane & labdane diterpenoid precursors follow polyene cyclization. Therefore, it is envisioned to synthesize both the naturally occurring dienophile and diene utilizing asymmetric polyene cyclization. The absolute configuration of (+)-taiwaniadduct J was unequivocally determined through the enantioselective synthesis and confirmed by X-ray crystallographic analysis This research highlights the effectiveness of employing pericyclic reactions, including the Diels-Alder[2] and [2+2] cycloadditions, for the efficient construction of intricate molecular frameworks, particularly those containing multiple quaternary stereocenters, as exemplified by taiwaniadduct J.

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Title: Unraveling Phase- and Sequence-Dependent Conformational Switching in Capped DPGX Tripeptides: A Combined X-ray Crystallography, Solution-Phase Spectroscopy, Gas-Phase Laser Spectroscopy, and Quantum Chemistry Study

Student Name: Sourav Mandal

Affiliation: IISER PUNE

Poster Code: 21

Abstract: The secondary structures of peptides, along with the strong propensities of specific amino acid sequences, play a pivotal role in determining the three-dimensional structures of proteins. Among these, β-turns are crucial as they reverse the direction of the polypeptide chain, facilitating the formation of compact, globular protein structures. These turns are particularly important for stabilizing β-hairpin motifs, which are essential for the overall stability and function of proteins. The ^{D}Pro-Gly sequence is widely recognized as a potent β-turn inducer in peptide antibiotics and peptidomimetics.[1] In this study, we investigated the secondary structures of the tripeptides Boc-^{D}Pro-Gly-Ala-NHBn-OMe (^{D}PGA) and Boc-^{D}Pro-Gly-Val-NHBn-OMe (^{D}PGV) using a combination of gas-phase laser spectroscopy, quantum chemistry calculations, solution-phase IR, 2D-NMR spectroscopy, and single-crystal X-ray diffraction (XRD). For ^{D}PGA, gas-phase laser spectroscopy and quantum chemistry calculations identified two low-energy conformers. The global minimum conformer adopts a type II′/I double β-turn structure, while the other exhibits a C7-C7-C7 conformation. Notably, the peptide structure obtained from FTIR, 2D-NMR and XRD closely matches the most stable type II′/I double β-turn structure observed in the gas phase.[2] Interestingly, when Ala was replaced with Val, we observed a conformational switch in the solid and solution phases, while the gas-phase structure remained similar. For ^{D}PGV, gas-phase laser spectroscopy and quantum chemistry calculations identified a single low-energy conformer, adopting a type II′/I double β-turn structure. However, in the solid and solution phases, ^{D}PGV formed a β-sheet structure, which significantly deviates from the most stable gas-phase conformation.[3] This divergence between gas-phase, solution, and solid-state structures highlights the fine interplay between intrinsic conformational preferences and external factors such as solvent interactions and crystal packing in determining peptide secondary structures. Gas-phase laser

spectroscopy uniquely identifies multiple low-energy conformations, providing insights into the intrinsic folding preferences of peptides. Understanding whether peptide folding is primarily governed by backbone hydrogen bonding, intrinsic residue propensities, or environmental effects is crucial for rational peptide design. These findings are particularly relevant for designing peptides with structural stability in both aqueous and hydrophobic environments, paving the way for advancements in therapeutic peptides, supramolecular assemblies, and biomolecular engineering.

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Title: Interstellar Phylogenetic Tree

Student Name: SHIVANI B

Affiliation: IISER TIRUPATI

Poster Code: 22

Abstract: Despite the extreme astrophysical conditions, our universe is chemically very rich and complex. This is quite evident as more than 300 molecules have been detected in the interstellar medium to date. Many of them are prebiotically relevant molecules, which form the foundation for life. Yet, the plausible chemical processes that shape interstellar chemistry are not well understood. In this backdrop, we envision that an “interstellar phylogenetic tree”, which works on the principle of descent with modification, shall offer a new framework for visualizing the complex interconnections between various molecular reactions in the interstellar medium. On this foundation, our study focuses on constructing a systematic and automation-friendly way to identify what reactions would aid in molecular evolution and what products may be feasible for further detection in the interstellar medium. Additionally, the constructed tree provides new avenues for future research into the chemistry of comets, meteorites, and planetary systems and could perhaps be relevant in aiding our grand goal of finding life beyond our planet

Title: Unlocking Selective Chloride Transport through EDTA-Induced Decomplexation of a Copper-Acylhydrazone System

Student Name: Umesh Shivpuje

Affiliation: IISER PUNE

Poster Code: 23

Abstract: The dynamic interaction between metal complexes and ethylenediaminetetraacetic acid (EDTA) as a chelating agent involves rapid and reversible processes of complexation and decomplexation. These processes provide a foundation for designing stimuli-responsive systems capable of regulating ion transport under specific environmental conditions. Such systems represent a versatile and tunable strategy for modulating transmembrane transport, with potential applications in controlled environmental sensing and biomimetic materials. In this study, a copper-based acylhydrazone complex was synthesized, which initially exists in an OFF state, exhibiting no ion transport activity. However, upon the introduction of Na_2EDTA as an external stimulus, the copper ions are selectively chelated, triggering the activation of the acylhydrazone moiety. This transition shifts the system to an ON state, enabling the selective and efficient transport of chloride ions across membranes. This work highlights the potential of metal-ligand interactions in developing responsive molecular systems for precise ion transport regulation, offering insights into the design of advanced functional materials.

Title: Precision Engineering Enabled Homogeneous Antibody-Drug Conjugates

Student Name: Sneha Basa

Affiliation: IISER BHOPAL

Poster Code: 24

Abstract: Antibody conjugates have emerged as transformative platforms for targeted therapies, revolutionizing diagnostics and treatment strategies. Antibody-drug conjugates (ADCs) combine the exquisite specificity of monoclonal antibodies (mAbs) with the potent cytotoxicity of therapeutic agents, thus delivering a precision-targeted therapeutic effect. The sophisticated assembly of a mAb, linker, and drug governs the ADC's pharmacokinetics, efficacy, and safety. To achieve the highly sought-after homogeneity in ADCs, the bioconjugation technology that links the drug to the mAb demands precise engineering.

We harnessed our in-house Linchpin Directed Modification (LDM®)[1] and Linchpin Directed Catalysis (LDC)[2] to modularly engineer the antibody, granting us unparalleled control over the homogeneity of the ADC. Moreover, linkers are indispensable in ensuring the ADC’s stability in the extracellular environment, its efficient intracellular release, and its systemic circulation time within the body. To regulate these vital properties, we have integrated a cathepsin B-cleavable valine-citrulline linker fused with polyethylene glycols (PEGs). Our chemical technologies also allow for the orthogonal installation of a hydroxylamine derivative of the toxin-linker, leading to the creation of precisely engineered ADCs. These constructs are likely to address the technological demands in the field and unlock the full potential of targeted therapy.

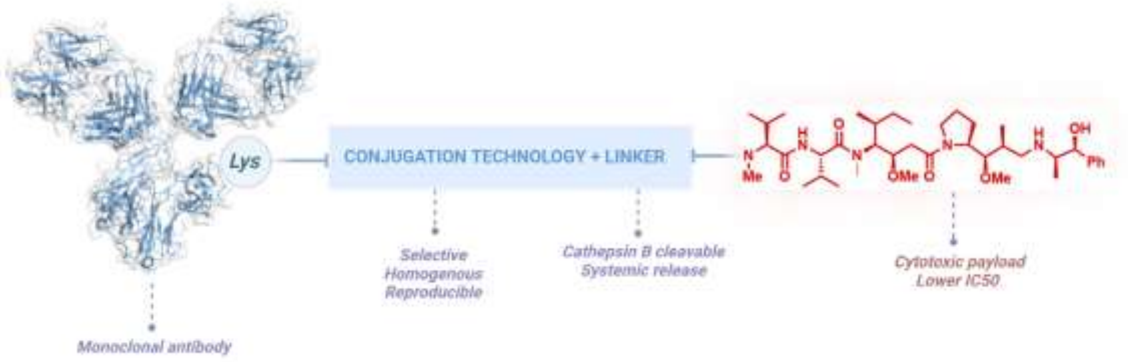

Figure. Homogeneous antibody-drug conjugates from LDM® and LDC platforms.

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Title: Leveraging Metaheuristics to Uncover Water Confinement in Multilayer Graphynes

Student Name: Megha Rajeevan

Affiliation: IISER THIRUVANANTHAPURAM

Poster Code: 25

Abstract: Global optimization is an effective method to study the geometries and energetics of atomic or molecular confinement in nanostructures. The high computational cost associated with modeling such complex chemical systems calls for the adoption of stochastic global optimization techniques. Herein, we employ a swarm intelligence-based technique, namely, particle swarm optimization (PSO)[1], to study the confinement of water clusters in monolayer and multilayer graphynes (GYs)[2], including ã-GY-2, ã-GY-3, and ã-GY-4. The water molecules are described using the TIP4P model[3]. The non-electrostatic part of GY-water and GY-GY interactions are modelled using the optimally fitted improved Lennard-Jones potential[4] and Hod's interlayer potential[5], while the Coulombic potential is employed to express the electrostatic interactions between GYs and water. Our PSO results reveal that the pore size of GYs plays a crucial role in the confinement of water clusters in multilayer ã-GYs. The ã-GY-2 multilayer tends to accommodate water as a monolayer between its two layers for large cluster sizes.[6] A single-file conformational motion of water molecules is observed when water clusters were confined within the ã-GY-3 trilayer. ã-GY-4, with the largest pore size, allowed clustering of water molecules within the pore pockets. The results established the importance of incorporating the twist features of GYs in the modelling formulation, as well as the accurate description of empirical formulations. Our findings set the groundwork for extended research on water transport through twisted multilayer GYs.

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Title: Biological Degradation of Graphitic Carbon Nitride Sheets and Autophagy Induction in Macrophages

Student Name: K. Swetha

Affiliation: IISER THIRUVANANTHAPURAM

Poster Code: 26

Abstract: The discovery of graphene has led to the exploration of numerous two-dimensional materials (2DM) increasingly used in industrial and biomedical applications. However, nano-safety and biological degradation are poorly understood.[1] Recently, the metal-free 2DM, graphitic carbon nitride (g-C_3N_4), has gained attention for its optical properties and potential applications in cancer therapies and bioimaging due to its low toxicity and fluorescence. In this regard, investigating the biodegradability of such materials will be crucial for understanding their in vivo fate and for designing potential biomedical applications.[2,3] Hence, we studied the biodegradability of two types of g-C_3N_4 nanosheets (exfoliated and porous) using human myeloperoxidase (hMPO, from neutrophils), plant enzyme HRP (horseradish peroxidase) and photo-Fenton reaction (PF, generating hydroxy radicals).[4] The biodegradation was followed by microscopic and spectroscopic techniques such as TEM, Raman, X-ray photoelectron, UV-vis and fluorescence spectroscopy. All these results confirmed that the g-C_3N_4 sheets could be degraded better by human enzyme (hMPO) over plant enzyme, HRP. Porous sheets showed higher degradability than exfoliated g-C_3N_4 sheets due to the presence of oxygen groups obtained during pre-acid treatment. Next, the PF reaction was performed to interrogate the degradation by-products using mass spectrometry, and the cytotoxicity of degradation products was assessed in comparison with pristine g-C_3N_4. Further, the impact of g-C_3N_4 on the induction of autophagy in the RAW264.7 macrophages was confirmed by over-expression of the autophagy marker, LC3 protein, significantly observed for the porous sheets. Finally, the immunomodulatory function of the nanosheets and cytokine production was also evaluated in RAW macrophages, demonstrating that the porous nanosheets induced a dose-dependent pro-inflammatory response. Autophagy induction highlights the potential use of g-C_3N_4, which could be applied in cancer therapies to induce suppressed autophagy.

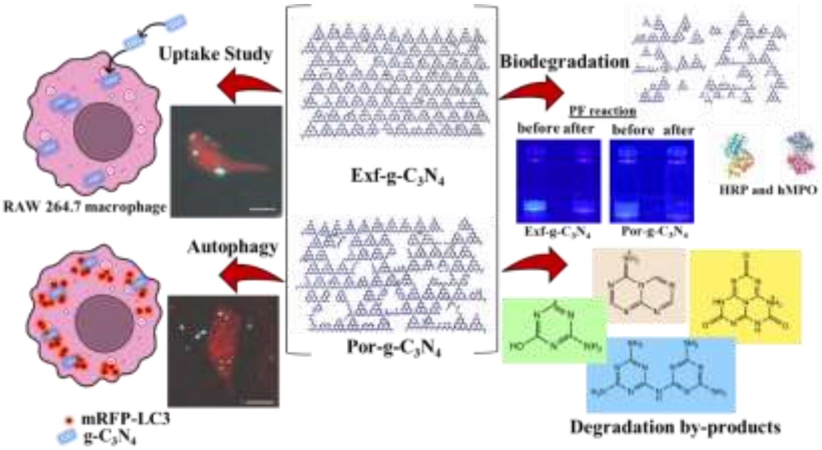

Figure 1. A representation of Exf and Por g-C3N4 degradation by hMPO, HRP and PF reaction. Degraded by-products after PF reaction (150 h) were studied and cellular uptake and impact on the autophagy in RAW macrophages were also examined after incubating with g-C_3N_4 sheets.[4]

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Title: Unprecedented Formation of Helical Macrocycle-Embedded with Pyrenyl Subunits

Student Name: Soniya Jacob

Affiliation: IISER THIRUVANANTHAPURAM

Poster Code: 27

Abstract: Expanded porphyrinoids constitute a class of compounds with larger ring size and extended ð-conjugation relative to naturally occurring tetrapyrrolic porphyrins[1]. Their conformational dynamics, governed by ring size and angular strain, afford a high degree of tunability in their physicochemical properties. This versatility enables the deployment of expanded porphyrinoids in diverse applications, including near-infrared (NIR) dyes, photodynamic therapy (PDT), magnetic resonance imaging (MRI) contrast agents, and nonlinear optical (NLO) materials[2]. In addition to these properties, the twisted conformations impart an intriguing characteristic to these macrocycles: chirality. Larger expanded porphyrinoids typically adopt *figure-eight* conformations due to angular strain and strong intramolecular hydrogen bonding interactions[3]. These *figure-eight* macrocycles are intrinsically chiral due to their inherent helical structure[4]. In this study, I will present the synthesis, structural characterization, and theoretical studies of a helical macrocycle **1** embedded with pyrenyl subunits. DFT studies predict a *figure-eight* structure for the macrocycle **1** in its free base form, which transforms into a box-like conformation upon protonation. Structural characterization of free macrocycle **1** was performed using MALDI, ^{1}H NMR spectroscopy, whereas the HOMO-LUMO gap and degree of aromaticity were evaluated using Kohn-Sham orbitals and NICS calculations, respectively. All the above studies will be presented in greater detail.

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Title: Low-Valent Chromium Catalyst for (De)hydrogenation reactions

Student Name: ABHIJITH K S

Affiliation: IISER TIRUPATI

Poster Code: 28

Abstract: The synthesis of useful N-containing building blocks by alcohols (De)hydrogenations is a highly selective and environmentally benign process. This method is applicable in sustainable chemical processes to overcome from traditional methods where water will be the sole by-product and alcohols used as alkylating reagents as well as hydrogen sources. Here, we report for the first time, a low valent chromium catalyzed C-N bond formations *via* borrowing hydrogen (BH) strategy to synthesize secondary amines. Our catalyst has the capability to tolerate multiple functional groups to give desired product good to excellent yields and thus an alternative to noble metals in (de)hydrogenation reactions. We used a catalytic amount of base as an additive and low cost TMEDA ligand for (De)hydrogenations. Deuterium labeling and control experiments supported our BH reaction mechanism and prepared secondary amines further functionalized to get *Tripelennamine* drug analogs to show the synthetic utility. Our findings further shows that the current low valent Chromium catalyst is capable enough to transfer hydrogenations (TH) for the synthesis of primary amines from corresponding nitro and nitrile compounds.

Title: Room Temperature Phosphorescence of Peptide Mimetic Luminophore

Student Name: Pradip Kumar Hansda

Affiliation: IISER KOLKATA

Poster Code: 29

Abstract: Room temperature phosphorescence (RTP) from peptide mimetic molecules represents an emerging area of research at the intersection of materials science, photo physics, and bioimaging. Recently, peptide mimetics have been engineered to exhibit RTP, a phenomenon where molecules emit light over extended periods after excitation, even at ambient conditions. This property is attributed to the suppression of non-radiative decay pathways and stabilization of triplet excitons through molecular design, such as incorporation of rigid structures, heavy atoms, or hydrogen bonding networks. RTP-active peptide mimetics offer unique advantages, including high sensitivity, long emission lifetimes, and biocompatibility, making them promising candidates for applications in bioimaging, optoelectronics, and anti-counterfeiting technologies.

The incorporation of aromatic residues, halogenation, and supramolecular assembly, may significantly enhanced RTP efficiency and lifetime. In this work we have incorporate electron deficient perfluoro aromatic moiety into the unconventional fluorophore backbone and fluorophore backbone itself exhibits an interesting photophysical and mechanoresponsive behaviour. Without direct conjugation between donor and acceptor a charge transfer can be achieved (Figure 1). Incorporating perfluoro-aromatic moiety this will helps to form self-assembled fiber type morphology through strong face to face pi-pi stacking and H-bonding. This is a new strategy to rigidify the system and it will suppress the nonradiative energy loss and stabilized the triplet energy state which leads a RTP from purely organic molecules. This work highlights the fundamental principles, design strategies, and potential applications of RTP in peptide mimetic systems with improving quantum yield.

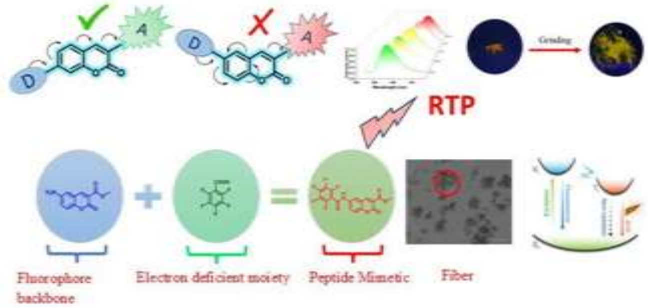

Figure 1. RTP of Peptide Mimetic Luminophore

Title: Exploring the Dielectric-Controlled Ultrafast Pathways in Push-Pull Stilbene through Global and Target Analysis

Student Name: Shaina Dhamija

Affiliation: IISER MOHALI

Poster Code: 30

Abstract: The twisted intramolecular charge transfer (TICT) process occurs in coplanar molecules with donor and acceptor moieties, where light excitation induces electron transfer, and a subsequent molecular twist prevents back electron transfer. This phenomenon originated from the observation of two fluorescence bands in 4-(dimethylamino) benzonitrile (DMABN), initially assigned to different polarities but later attributed to excited-state species with different orientations of the donor and acceptor groups[1]. Some push- pull stilbenes, have attracted significant attention due to their interesting photophysics, where on one hand like 4,4’-dimethylaminocyanostilbene (DCS) exhibits increase in fluorescence quantum yield

(QY) on increasing the solvent polarity, however, 4,4'-dimethylaminonitrostilbene (DNS)[3] shows an increase in fluorescence QY on increasing solvent polarity but it decreases at very higher polarities of solvent, which can be possibly due to competing relaxation pathways like TICT or isomerization. In the present work, we investigated the ultrafast excited-state dynamics of DNS in different polarity solvents by employing femtosecond transient absorption spectroscopy (fs-TAS). Single-wavelength kinetic analysis of fs-TAS data often show overlapping signals from different species and processes, making it challenging to resolve individual contributions. Therefore, we employed global and target analysis to isolate excited species involved in these photoexcitation-induced processes by fitting across all wavelengths and time points, to unveil mechanistic details on twisting versus isomerization processes.

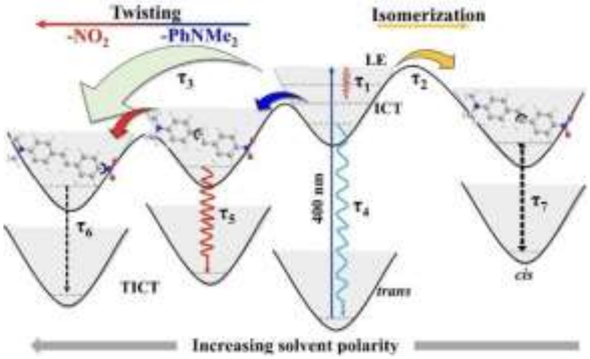

Figure 1. Proposed schematic depicting structural changes in excited-states with change in solvent polarity showing twisting versus isomerization pathways.

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Title: Rectangular Porphyrin Carbazole Cages for Encapsulation of Fullerenes

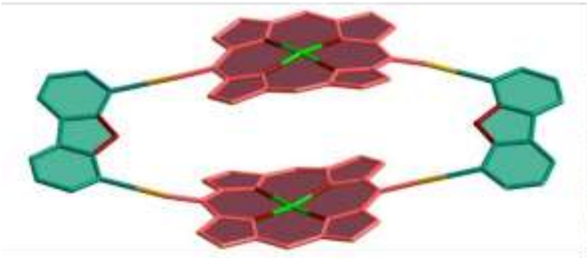
Student Name: Mohini Mittal

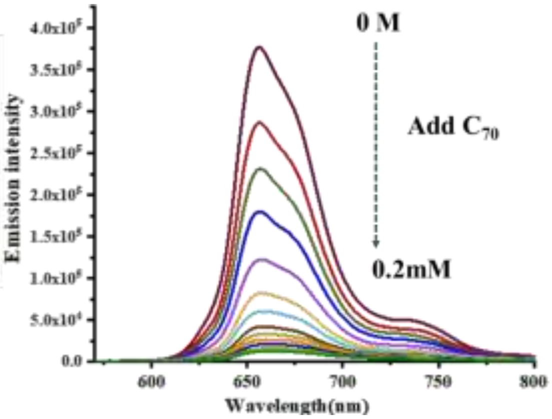
Affiliation: IISER BHOPAL

Poster Code: 31

Abstract: Three-dimensional (3-D) molecular cages that are shape-persistent, covalent organic polyhedrons (COPs) with well-defined pore dimensions, have received much attention for their multiple applications in host-guest chemistry, catalysis, organic solar cells, etc.[1] Fullerene has sparked intense research interest due to their unique electron-accepting properties and applications in photovoltaics, electronics, and biopharmaceutical industries.[2] However, the difficulties in purifying, solubilizing, and derivatizing fullerenes can be overcome through p-electronic donor-acceptor interactions during complexation in host-guest chemistry. Electron-rich molecules such as porphyrins and polycyclic aromatic hydrocarbons can be used as hosts for fullerene encapsulation by non-covalent interactions due to their large p-surface. In this direction, fullerene-selective receptors with diverse geometric shapes of cavities have been discovered, such as molecular cages,[3,4] nanotubes,[5] and cavitands,[6] etc. Herein, we intend to create a smaller porphyrin cage with the optimum cage size and rigidity to bind fullerenes with high affinities and selectivity.

In this talk, we will discuss the synthesis of rectangular porphyrin dimer using 3,6-di-tert-butyl-1,8-diethynyl-9H-carbazole (Cbz-CH), Cbz-CH acts as a short spacer, which leads to the formation of a smaller cavity. Further, we will discuss how these dimers act as receptors for fullerenes (C_{60} and C_{70}) through non-covalent interactions.





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Title: Spatial tuning of biocondensate forming zone in a microfluidic gradient of dissipative condition

Student Name: Sakshi Juneja

Affiliation: IISER MOHALI

Poster Code: 32

Nature utilizes dissipative self-assembly to regulate crucial biological processes as it enables the formation of complex dynamic structures that exist under non – equilibrium conditions. Reproducing this non-equilibrium chemistry in vitro with (bio)molecules is crucial for the design of life-like dynamic materials that emerge through a continuous flux of energy [1]. Herein, we observed the spatial tuning of biocondensates of DNA- histone (which are membrane-free micron-scale organelles formed by multivalent interactions between biomolecules) [2] under dissipative conditions by introducing chemical fuel (histone) and a fuel-degrading agent (trypsin) into Y-shaped microfluidic chip under flow condition and the self-assembly was sustained under NESS conditions. We found that under dissipating conditions the drift of the biocondensates is towards structure forming zone or fuel-rich zone and the drift of the structure-forming zone can also be controlled by adjusting the flow rate in the microfluidic setup. Additionally, we observed that the transport of the catalyst (DNAzyme) and its associated zonal reactivity can be modified by using this system [3].

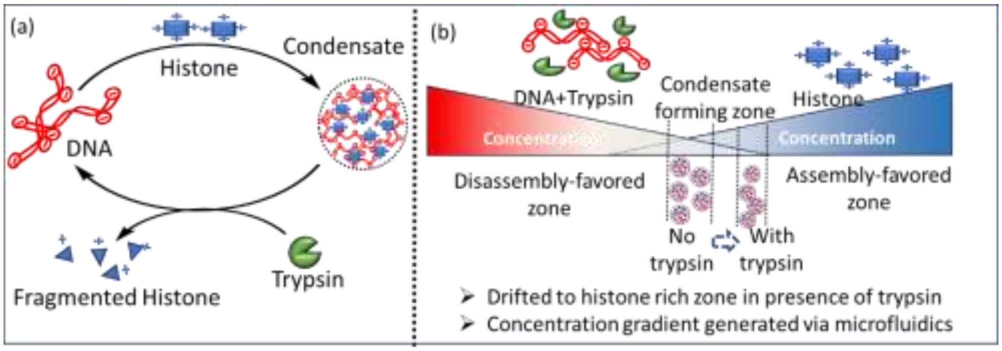

Figure 1. (a) Schematic representation of DNA-histone condensate and its dissociation due to fragmentation of histone by trypsin. (b) Schematic showing the formation of DNA-histone condensate at the meeting point of their gradient, however condensate forming zone shifted towards histone-rich side in presence of DNA + trypsin gradient.

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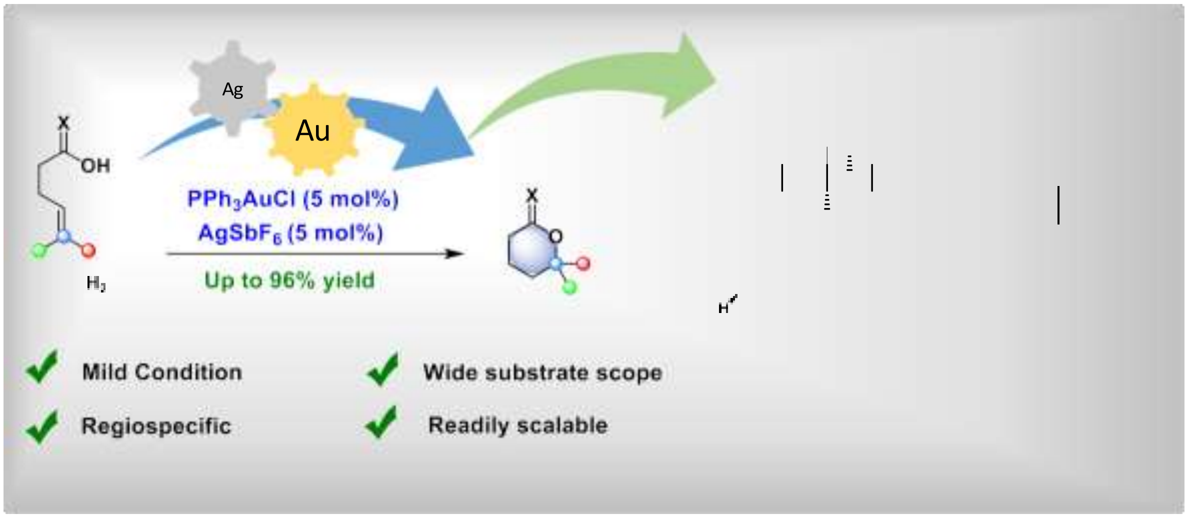
Title: Dual Au/Ag Catalyzed Regiospecific Intramolecular Hydroacyloxylation and Hydroalkoxylation of Unactivated Geminal-Substituted Olefins.

Student Name: AKASH DHURI

Affiliation: IISER TIRUPATI

Poster Code: 33

Abstract: A mild, regiospecific Gold-Silver bimetallic catalytic system has been devised for the intramolecular hydroacyloxylation and hydroetherification of alkenoic acids and alcohols. This method exhibits precise specificity for the geminal substituted olefinic center and facilitates the synthesis of substituted phthalide and hydroisocoumarin derivatives. This method has been effectively applied for late-state functionalization to produce bioactive natural products such as mycophenolate and in the synthesis of rumphellaone A and (−)-ambrox. The successful gram-scale synthesis of the anticonvulsant, hypnotic drug (±)-ethyl phenyl butyro lactone (EPBL), (±)-Boivinianin A and the ability to synthesize challenging spiro and bicyclic lactone underscores the synthetic potential of this methodology. Mechanistic insights into gold-silver catalyzed lactonization of olefins have also been discussed.



Title: "Exclusive pathway selectivity of dimorphic aggregates in an n-type semiconductor: Distinct optical properties and electron mobility"

Student Name: SHREYA TYAGI

Affiliation: IISER PUNE

Poster Code: 34

Abstract: The presence of polymorphic phases in crystalline domains and diverse aggregation pathways leading to distinct aggregated structures, along with isothermal phase transformations, poses a significant challenge in controlling the optical and electrical conductivity of bulk organic films—especially in molecular semiconductors. A low activation barrier between these equilibrium states of aggregates allows phase oscillation under thermal fluctuations during device operation, often resulting in inconsistent performance. Achieving selective aggregation through a top-down approach in solid-state or bottom-up pre-aggregation strategies and minimising phase crossover through significant thermal activation necessitates a precise understanding of structure-property correlations. Here, we present a robust example for achieving high domain purity in top-down and bottom-up trails using an *n*-type molecular semiconductor with dimorphic aggregates. This approach yields homogenous films with high field-effect electron mobility (~0.95 $cm^2V^{-1}s^{-1}$) in solution-processed OFETs, along with an excellent on-off current ratio ($I_{ON/OFF}$ ~ 10^8) and attractive device reproducibility. A detailed structural and mechanistic analysis offers a rare example of controlled aggregate formation on substrates. This work paves the way for more efficient organic electronic devices and holds potential for developing programmable ink formulations for next-generation electronics.

Title: 2-Mercapto Malonatesdiester Generate Hydropersulfides and Metabolically Integrated Byproducts

Student Name: Arnab Makhal

Affiliation: IISER PUNE

Poster Code: 35

Abstract: Hydropersulfides (RS-SH) are key mediators of several biological processes and along with hydrogen sulfide (H_2S) are considered among the first responders to perturbations of redox homeostasis.[1] Persulfides in cells have several direct and indirect effects such as activation of antioxidant signaling pathways, protection from lipid peroxidation, and mitigation of inflammation.[2,3] Hence, being able to generate persulfide in a controlled manner is important[4,5], both from a redox biological mechanistic understanding as well as possible therapeutic applications. Here, using fundamental acid-base chemistry, we developed 2-mercapto malonatediester as a generator of persulfide (RS-SH), through a direct sulfhydryl group (SH) transfer to thiols (RSH). The byproduct of this reaction is malonate, which is fully biocompatible since it is a component of fatty acid biosynthesis.[6] 2-mercapto malonatediester reacts with glutathione (GSH) and produce glutathione persulfide (GS-SH), a key antioxidant biomolecule that is involved in quenching of lipid radicals that contribute to cellular dysfunction and degeneration. This transformation gave the malonatediester in quantitive yield, underscoring the high efficiency of persulfide generation. Generation of GS-SH was also seen in cellular lysate, supporting the applicability of this probe for cell-based studied. Taken together, 2-mercapto malonatediesters generate persulfide and fully biocompatible byproducts, and can be used to promote antioxidant response with no trace left behind. Studies to evaluate anti-oxidant potential are underway.

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Title: Hypoxia Activated Prodrugs (HAPs) and their Targeted Release in Tumor Microenvironment

Student Name: PRAKASH SHUKLA

Affiliation: IISER BERHAMPUR

Poster Code: 36

Abstract: Different potent bioactive molecules often face severe challenges as therapeutics due to their cancer cell resistance, poor bioavailability, and unintended toxicities which restrict them from reaching the final drug approval[1]. Different strategies have taken up to circumvent these challenges. Prodrug synthesis is one of the major avenues often utilized where the active molecule is masked with the attachment of functionalities by a tailor-made synthetic approach[2]. However, early degradation and non-specificity still remain with the newly developed prodrugs[3]. Hence, to achieve a more targetable approach, we have designed hypoxia-activatable prodrugs by functionalizing a potent bioactive molecule β-lapachone by attaching a hypoxia-responsive diazo linkage. Under the tumor microenvironment, the diazo bonds will be cleaved in a reducing medium followed by a low pH activatable release of the potent molecule via C-C bond cleavage, specifically releasing the potent molecule in the tumor site owing to lesser side effects. Electronic effects on the prodrug molecule have been varied by he virtue of functionalization to achieve better stability and sustained release profile and it has been found that by attaching electron withdrawing groups the prodrug achieve extended stability and the release gets facile under tumor mimic conditions. Facile release and higher tolerated dose is observed under in vivo setup which highlights the importance of strategic design. This molecule can provide a highly potent and alternative approach for designing prodrugs of active chemotherapeutic molecules, although therapeutic efficacies are yet to be performed to demonstrate the system as a modern example of a tumor-specific prodrug scaffold.

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Title: Recovering Maximum Exciton Energy by Hot-Exciton Channel of Organic Donor-Acceptor Based HLCT Emitters: Development of Highly Efficient Non-Doped OLEDs

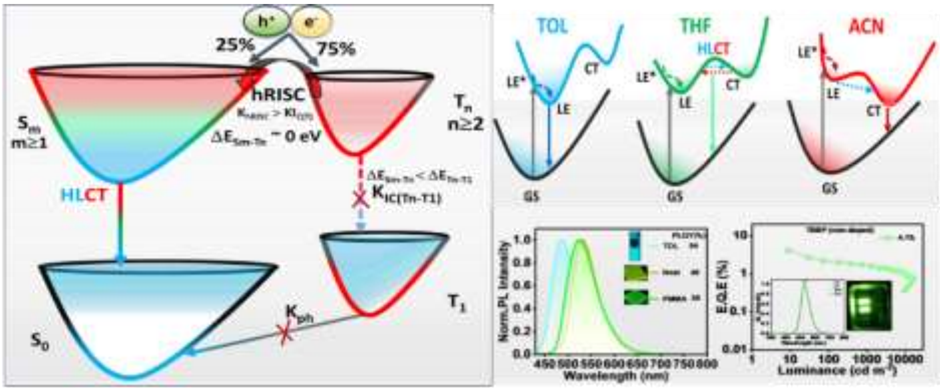
Student Name: Sk Samsul Ghaus

Affiliation: IISER KOLKATA

Poster Code: 37

Abstract: Hybridized local and charge transfer (HLCT) based fluorescent emitters are outstanding candidates for organic light-emitting diodes (OLED) owing to their excellent performance in exciton utilization energy (EUE) and highly efficient color-tunability. HLCT technology is used to develop more energy-efficient displays with improved visibility of output light to create next-generation OLED. However, the inherent mechanism of HLCT-based fluorescent emitters was still unclear and need better understanding. Herein, we propose a detailed mechanistic description for HLCT-based fluorescent emitters using solvatochromism, temperature-dependent measurements, theoretical evidence and substantiated with fs-transient absorption spectroscopy (fs-TAS). We have synthesized three novel D-ð-A systems with triphenylamine (TPA) linked electron donor and benzophenone derivatives (substituted one benzene ring by thiophene group), which act as acceptors (with acronym TSBP, TBPS and 2TBPS). All of these compounds exhibit very good quantum yield in solution and film states. TSBP shows better results due to its high quantum efficiency (Ö$_{\mathrm{PL}}$= 94% in toluene, 40% in neat film and 85% in PMMA-doped film). We observed a shift in the locally excited (LE) energy state to hybridized local and charge transfer (HLCT) state and subsequently to charge-transfer (CT) state in non-polar (toluene) to medium polar (THF) to strongly polar (ACN) solvents. Kinetics of the process was clearly understood from fs-TAS. These fluorescent emitters fabricated highly efficient OLEDs (green-emitting in non-doped and cyan blue-emitting in doped). These OLEDs were prepared using a simple solution processable method using conventional device architecture. TSBP shows significantly better results in non-dopped as

well as doped (7 wt% CBP host) conditions as this emitter reaches a maximum current efficiency (CE_{max}) of 15.4 cdA^{-1}, power efficiency of 13.8 lm W^{-1} and maximum external quantum efficiency (EQE_{max}) of 4.1% in non-doped system with the CIE coordinates of (0.28,0.62) and 5.6% in the doped system with the CIE coordinates of (0.20,0.55).



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Title: Resonance Plasmonic Coupling for Selective Band-Edge Emission in Semiconductor Quantum Dots

Student Name: Livin Paul

Affiliation: IISER THIRUVANANTHAPURAM

Poster Code: 38

Abstract: The semiconductor quantum dots (QDs) with size tunable emission make them a promising candidate for optoelectronic applications. However, undesirable nonradiative decay pathways of excitons reduce their emission quantum yield and colour purity. The emission properties of QDs are often enhanced by eliminating the surface trap states through chemical methods.[1,2] The spontaneous emission of an emitter is not an inherent property; rather, it varies with the local electromagnetic or photonic environment. The modification in the photonic environment can be achieved by the resonance plasmonic coupling.[3] Here we presents a physical approach to improving emission purity in QDs using frequency-specific plasmon resonance coupling.[4] By electrostatically binding negatively charged CdSe QDs to positively charged gold nanoparticles with a thin polymer coating, we achieve selective enhancement of band-edge emission. At a lower emitter density, a selective enhancement of band-edge emission over trap-state emission is observed and the emission enhancement factor closely follows the plasmon

resonance. However, at higher densities, nonradiative energy transfer leads to quenching, indicated by a redshift in the emission spectrum.

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Title: Synergistic behaviour of SLS-Triton X 100 at their CMC

Student Name: RONIT GAURANG SHETH

Affiliation: IISER PUNE

Poster Code: 39

Micellization behavior of the binary mixture of sodium lauryl sulfate (SLS) and Triton X-100 was studied using the dye solubilization method and curcumin as the hydrophobic dye. Adsorption behavior was studied, and Rubingh's model of non-ideal behavior was used to calculate the interaction parameters of the system. Synergism effects, observed in the mixture of surfactants, resulted in increased solubilization of the dye and a noticeable decrease in the critical micelle concentration (CMC). Micellization and adsorption behavior of the mixture were also nearer to that of Triton X-100 compared to SLS, regardless of composition. CMC reduction is especially useful in most industries because lower concentrations of surfactant result in greater efficiency, cost savings, and lower environmental impacts; such industries are pharmaceutical drug delivery, detergency, personal care products, enhanced oil recovery, wastewater treatment, and textile processing. Azeotropic behavior at a certain composition with stable micellar structure over a wide concentration range was also observed for the mixture.

Title: Microscopic Understanding of Dynamic Catalysis Using a Discrete-State Stochastic Approach.

Student Name: Pankaj Jangid

Affiliation: IISER PUNE

Poster Code: 40

Abstract: Dynamic catalysis, a phenomenon where the catalytic properties of a system change over time, stands in stark contrast to static catalysis, where the catalytic activity remains constant. This exciting concept has gained attention as a potential alternative to traditional static catalysis, with the expectation that it could significantly improve catalytic efficiency, promising an alternative to static catalysis.[1] The dynamic restructuring of active sites on the surface has been observed in nanocatalysts, which refers to the ability of the surface to change its atomic rearrangement.[2] Thermal isomerization of nanocatalysts and nanoclusters can result in a diverse array of catalyst structures with differing activity.[3] The microscopic mechanisms underlying these processes are poorly understood, posing a challenge to researchers aiming to exploit and control these phenomena for improved catalytic performance. We have developed a novel stochastic framework that enables the quantitative characterization of dynamic catalysis, facilitating a comparison of its properties with those of the static approach.[4] Observations indicate that fluctuations between distinct catalytic pathways can result in improvements in chemical reaction rates, albeit within specific ranges of kinetic parameters. We show that the temporal efficiency of dynamic catalysis depends only on the rates of chemical reactions and transitions between different catalytic pathways while being independent of the number of active sites. Dynamic catalysts operate outside of equilibrium conditions, and the energy dissipation associated with this dynamic behavior is a crucial factor driving improvements in catalytic efficiency. We further examine how temperature influences the dynamic efficiency of the catalyst. Depending on the activation energies of the catalyst, temperature can either enhance or reduce its efficiency. In addition, the stochastic aspects of dynamic catalysis have been studied which emphasizes the importance of considering probabilistic elements in the analysis of dynamic catalytic reactions. Our theoretical method can explain these observations from the microscopic point of view and may be helpful in building better catalysts.

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Title: Pd/Brønsted acid catalysed atom-economical [3+3] annulation of 4-hydroxycoumarins and skipped enynes

Student Name: BHAVYA KHAITAN

Affiliation: IISER BERHAMPUR

Poster Code: 42

Abstract: We report a [3+3] annulation of skipped enynes with 4-hydroxy coumarins, which gives a completely atom-economic synthesis of fused O-heterocycles. The unique feature of skipped enynes as bis-electrophiles under Palladium/Brønsted acid catalysis is explored. The proposed reaction pathway is via the Pd-catalysed C-H activation of the skipped enyne, which leads to a diene, which upon successive activation by Pd and nucleophilic attack by O, leads to the regioselective formation of pyrans containing a vinyl substituent

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