VISION

2030

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Indian Institute of Technology Guwhati
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Research Area

- Supramolecular Chemistry
- Material Chemistry
- Theoretical Chemistry
- Physical Chemistry
- Biological Chemistry
- Organic Chemistry
- Inorganic Chemistry

Content

Hypermolecular Interaction - Based Molecular Superlattices in Two Dimensions

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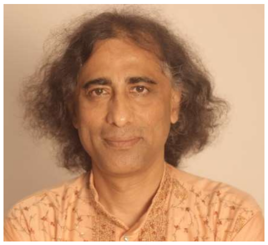

We are interested in pursuing assemblies of molecules into two-dimensional lattices and subsequent generation of higher order structures by careful superpositions of the constituent lattices. We are particularly focused on moiré superlattices where the constituent lattices would be stacked angularly against each other. Our observations suggest that the stackings at low angles (say, at 1 to 5^0) generate moiré and/or super-moiré superlattices that have novel chemical, optical and electrical properties, which are not available with the ordinary lattices. We have defined and proposed that the new properties that arise out of the super-assembly may be due to hypermolecular van der Waals and non-van der Waals interactions at the interfaces of the constituent lattices. We are also keen on pursuing hetero-structured superlattices where the component lattices would be based on different chemical identities.

We are further interested in investigating novel physical phenomena involving matter at the nanoscale. For example, we have recently discovered, using surface-enhanced Raman spectroscopy, that the well-known "coffee ring" deposition from gold nanoparticle dispersion - at the three-phase contact line (TPCL) of an evaporating sessile droplet - occurs via a phase-transition. Similarly, we could distinguish intra-nanoparticle versus inter-nanoparticle plasmon-enhanced chemical reaction rates by pursuing the reaction at the TPCL.

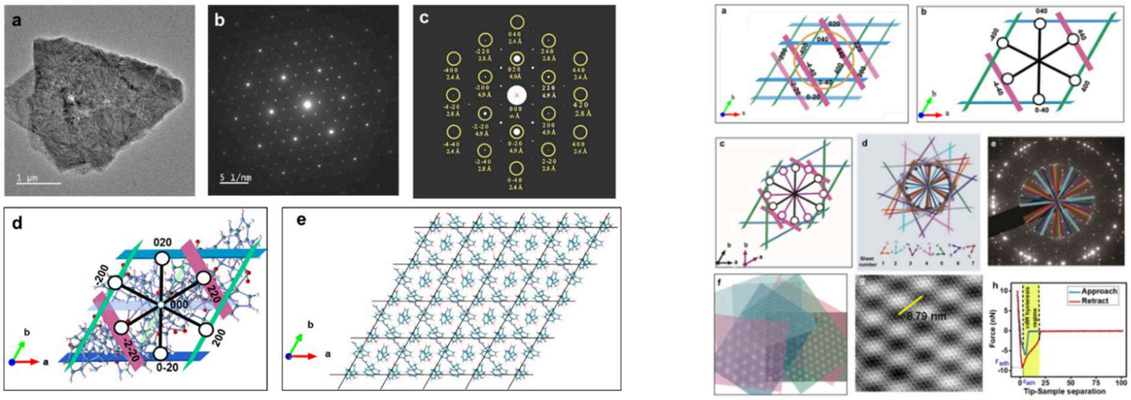

Figure: Moiré superlattice formation of tryptophan molecules. Refer to [1] for further details.

1. Two-dimensional Molecular Moiré Superlattices of Tryptophan with Visible Photoluminescence for Photo-activatable CO_2 Sensing and Storage. Ujjala Dey and Arun Chattopadhyay. ***J. Mater. Chem. C.* 2024**, DOI: 10.1039/D4TC00050A.
2. Moiré Superlattices of Two-dimensional Copper Nanocluster Assemblies with Tuneable Twin Emissions from Hierarchical Components Leading to White Light Emission. Priya Das and Arun Chattopadhyay. ***J. Mater. Chem. C.* 2023**, DOI: 10.1039/D3TC02193A.
3. Enhanced Chemical Stability in the Twisted Dodecagonal Stacking of Two-Dimensional Copper Nanocluster Assemblies. Priya Das and Arun Chattopadhyay. ***J. Phys. Chem. Lett.* 2022**, DOI: 10.1021/acs.jpclett.2c02300.
4. Chemically Reversible Translational Moiré Superlattice Formations in the Two-Dimensional Films of the Zinc Phthalate Complex. Archismita Hajra and Arun Chattopadhyay. ***J. Phys. Chem. Lett.* 2024**, 15 (39), 10046–10053.
5. Moiré Superlattices of Zn^{2+} Mediated 2D Assembly of Mn^{2+}-Cysteine Complex Nanoparticles Alter Electron Spin Transitions in the X-band. Archismita Hajra and Arun Chattopadhyay. ***Chem. Mater.* 2024**, 36 (17), 8523–8533.
6. Distinction of Plasmonic Intrananoparticle and Internanoparticle Molecular Reaction Rates at the Three-Phase Contact Line of an Evaporating Sessile Droplet. Sujay Paul and Arun Chattopadhyay. ***J. Phys. Chem. Lett.* 2024**, 15 (26), 6812-6817.

Organic Synthesis and Catalysis Laboratory

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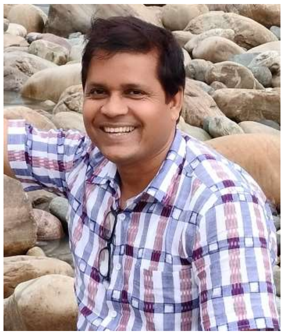
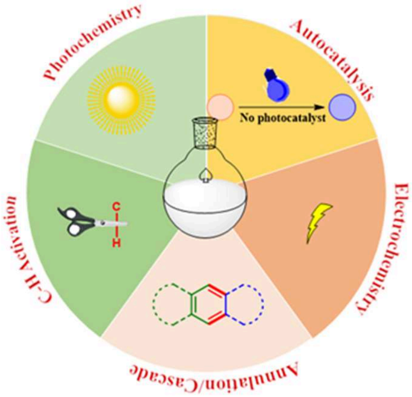


Our group would make further contributions in the area of Organic Synthesis focusing particularly on catalysis covering photo-, electro-metal, and metal-free protocol. Emphasis will be to construct organic molecules with potential applications in pharmaceuticals and materials science. Efficient use of photo- and electro-induced processes to facilitate environmentally benign and efficient synthesis of structurally complex molecules with high precision and functional group tolerance. To investigate mechanistic insights, and enrich the understanding of photo and electro-induced synthesis, providing useful information for future studies.



Developing luminescent materials, particularly AEEgens, and demonstrates the successful blend of organic synthesis, photophysical characterization, and biological applications. Fine-tune emission properties through structural modifications and exploration of their multifunctional use such as mechanochromic, bioimaging, forensic science, and biomedicine applications and making their practical use. Our study's emphasis on sustainability and its potential applications in drug development and material science sets a promising direction for future research in this field. Finally, developing photo degradation of functionalized non-biodedgadable polymers and converting them to useful product creating waste to wealth. The move toward more sustainable and efficient catalytic processes, also aligns with the broader goals of green chemistry, emphasizing the role of chemistry in contributing to sustainable development.

References:

(1) Khandelia, T.; Ghosh, S.; Panigrahi, P.; Mandal, R.; Boruah, D.; Patel, B. K*. Photo-induced 1,2-thiohydroxylation of maleimide involving disulfide and singlet oxygen. ***Chem. Commun.*** **2023**, *59,* 11196.

(2) Panigrahi, P.; Ghosh, S.; Khandelia, T.; Mandal, R.; Patel, B. K*. Isoxazole as nitrile synthon: en routes to the ortho-alkenylated isoxazole and benzonitrile with allyl sulfone catalyzed by Ru(II). ***Chem. Commun.*** **2023**, *59,* 10536.

(3) Dhara, H. N.; Rakshit, A.; Barik, D.; Ghosh, K.; Patel, B. K.* Visible-light driven electron-donor-acceptor (EDA) complex initiated synthesis of thio-functionalized pyridines. ***Chem. Commun. 2023***, *59*, 7990.

(4) Chakraborty, N.; Rajbangshi, K.; Dahiya, A.; Das, B.; Vaishnani, A.; Patel, B. K.* NIS-initiated photo-induced oxidative decarboxylative sulfoximidation of cinnamic acids. ***Chem. Commun.*** 2023, *59*, 2779.

(5) Khanddelia, T.; Ghosh, S.; Patel, B. K.* Dearomative bis functionalization of quinoxalines and bis-N-arylation of (benz)imidazoles via Cu(II)-mediated addition of boronic acids. ***Chem. Commun.*** **2023**, *59*, 2118.

(6) Das, B.; Dahiya, A.; Chakraborty, N.; Patel, B. K.* Synthesis of chromeno-pyrroles (azacoumestans) from functionalized enones and alkyl isocyanoacetates. ***Org. Lett.*** **2023**, *25,* 5209.

(7) Ghosh, S.; Khandelia, T.; Panigrahi, P.; Mandal, R.; Patel, B. K.* Mn(I) Catalyzed Preferential Electrophilic C3-Maleimidation in Quinoxaline Leading to Spiro-cyclization and Dehydrogenation of Succinimides. ***Org. Lett.*** **2023**, *25,* 3806.

(8) Rajamanickam, S.; Saraswat, M.; Venkataramani, S.; Patel, B. K.* Intermolecular CDC Amination of Remote and Proximal Unactivated Csp 3–H Bonds Through Intrinsic Substrate Reactivity – Expanding Towards a Traceless Directing Group. ***Chem. Sci.*****, 2021**, *12*, 15318.

Developing New Trends towards Modern Organic Synthesis

Dr. Tharmalingam Punniyamurthy

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The incessant identification of heterocyclic compounds in a broad spectrum of natural products and pharmaceuticals demands for the development of annulation strategies towards their comprehensive synthesis. Contextually, strained ring systems owing to their inherent simplicity and staple architecture find widespread application as viable building blocks in synthetic organic chemistry. In this realm, cycloaddition as well as ring-opening/cyclisation of strained rings act as the mainstay towards constructing complex molecular architectures due to their inherent ability to act as a 1,3-dipole in presence of Lewis acids. Further, achieving stereospecific cascade C-C and C-heteroatom bond formation, depicts excellent chirality transfer of our reaction methodologies. Asymmetric induction in cycloaddition to obtain stereoselectivity via the use of chiral ligands stands out as a major contributing factor towards achieving cost-effective protocol. Furthermore, we aim towards performing late-stage diversifications of our methodologies in addition to in-depth study from the mechanistic point of view. As an effort towards expanding our future scope, we also plan for exploring the utilities of strained ring systems in the field of photochemistry as well as energy transfer (EnT) reactions. In addition, merging electrochemical pathway with the chemistry of strained rings is our foremost objective to be exploited in the near future.

The C−H activation has emerged as a powerful transformative synthetic tool for editing and building complex molecular scaffolds which are ubiquitous in pharmaceuticals, agrochemicals, dyes, polymers, and many more and have even considered as a "***Holy Grail***" of chemistry for their step efficiency and atom economy. However, reactivity and selectivity, arising from the inertness of C-H bonds and their overabundance in organic molecules, are the two major fundamental challenges. In this regard, our laboratory, is fascinated by the prospect of selective C-H functionalization of benzo-fused *N*-heterocycles as well as construction of synthetically important multi-ring heterocyclic scaffolds in one step. However, in contrast to, *ortho* C-H activation, distal C−H activation remained a great synthetic challenge due to the inaccessibility of these sites in the formation of energetically favorable organometallic pretransition states. Furthermore, inception of photocatalysis in the C-H activation reaction have gained much attention in recent time, offering a sustainable alternative to the existing reaction methodologies. In this realm, our next plan is to devote more efforts to developing photo-induced remote C-C bond formation via cascade C-H Activation/C-C cleavage.

References:

1. Mishra, M.; Verma, K.; Banerjee, S.; Punniyamurthy, T. ***Chem. Commun***., **2024**, *60*, 2788.
2. Kar, S.; Maharana, P. K.; Punniyamurthy, T.; Trivedi, V. ***Org. Lett***., **2023**, *25*, 8850.
3. Bhattacharyya, H.; Saha, S.; Verma, K.; Punniyamurthy, T. ***Org. Lett***., **2023**, *25*, 6830.
4. Paul, T.; Basak, S.; Punniyamurthy, T. ***Org. Lett***., **2022**, *24*, 6000.
5. Karjee, P.; Mishra, M.; Debnath, B.; Punniyamurthy, T. ***Chem. Commun***., **2022**, *58*, 8670.

Chiral Recognition and Engineered Polymer

Dr. Manabendra Ray

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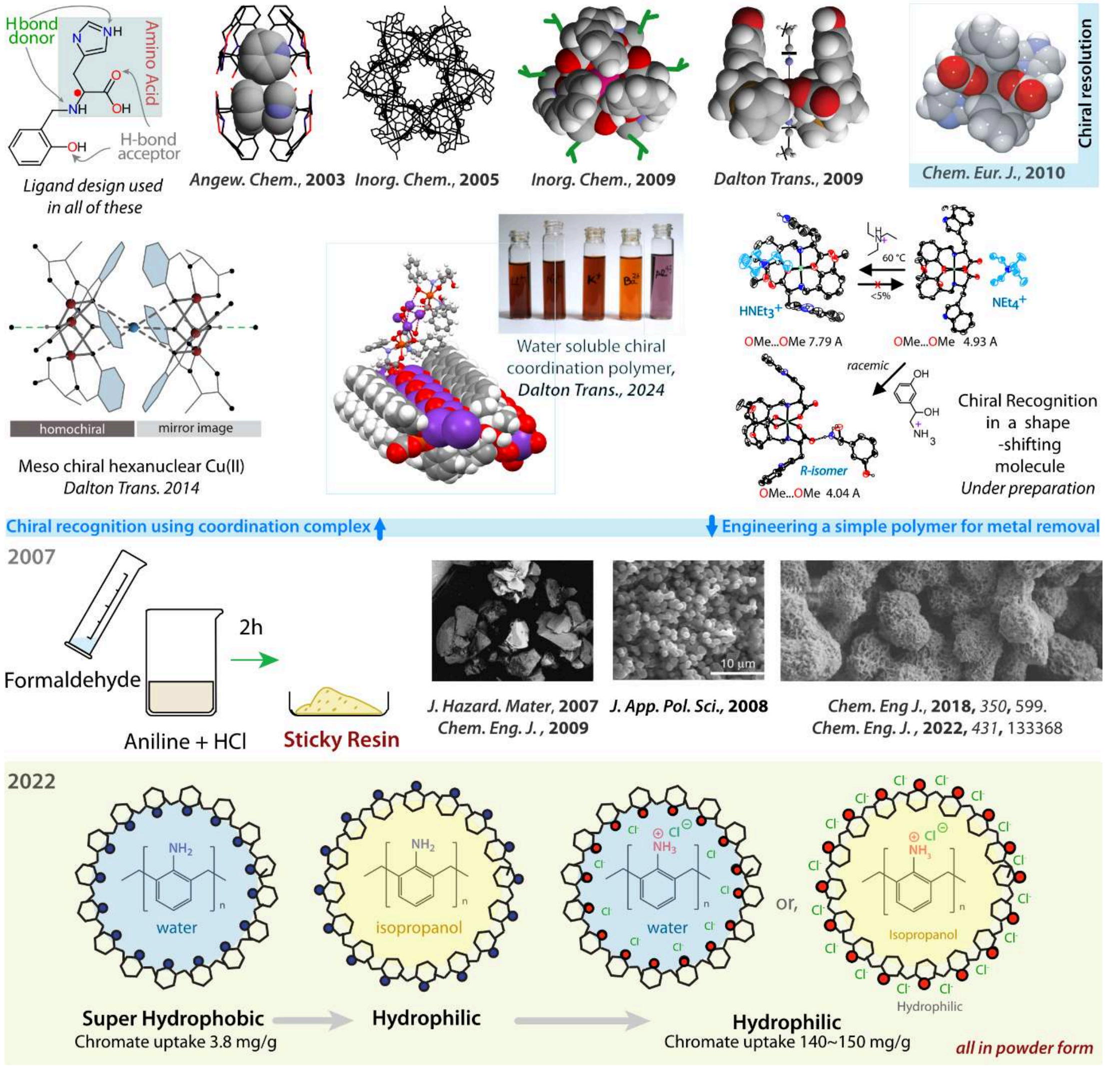
We started by designing a flexible amino acid-based ligand with the intention of addressing the problem of chiral recognition through non-covalent interactions as it happens in biology. More specifically, the target was adrenaline or other similar chiral amino alcohols. Our initial efforts were to make large chiral assemblies with cavities or channels, but eventually, we shifted to smaller molecules with binding pockets. The first success occurred in 2010. We are continuing by redesigning more versatile anionic chiral hosts. Parallely, we also started working on polymers capable of binding metals from industrial waste water. The focus here is to engineer a simple polymer to different architectures to increase efficiency and understanding of the binding at the molecular level.



Both the progress and the way forward are shown in the timeline above.

Heterocyclic Compounds of Biological Importance

Prof. Anil K. Saikia

Nitrogen, oxygen, and sulphur heterocyclic compounds have undoubtedly attracted the interest of synthetic chemists due to their occurrence in many natural products, pharmaceuticals, and smart materials. The development of novel highly efficient procedures for synthesizing these molecules is of current interest. These procedures must be compatible with our environment and should have economic advantages. In such an approach the reduction of several steps and increase in selectivity is a valuable standard for the quality of a synthesis. A general way to improve synthetic efficiency is the design of a selective transformation either in a diastereoselective or enantioselective fashion. Therefore, the development of methodologies for the synthesis of these molecules in a single step in stereoselective and environmentally friendly manner is one of our goals.

Although enormous methods are available in the literature for the synthesis of small and medium-ring heterocycles, the synthesis of large-ring heterocyclic compounds is a challenging task due to the instability of the large rings. Our main focus is to develop some new methodologies for the stereoselective synthesis of large-ring heterocyclic compounds of biological importance in a single step in an environmentally friendly atmosphere.

References:

1. Bikoshita Porashar, Bipin Kumar Behera, Hunmoina Phukon and Anil K. Saikia, ***Chem. Commun*. 2024,** *60*, 4358–4361.

2. Subhamoy Biswas, Sudip Shit, Bipin Kumar Behera, Archana Kumari Sahu and Anil K Saikia, ***Chem. Commun*. 2023**, *59*, 14301–14304.

3. Bikoshita Porashar, Subhamoy Biswas, Archana Kumari Sahu, Archana Chutia, and Anil K Saikia, ***Org. Lett*. 2022**, *24*, 9038–9042.

4. Subhamoy Biswas, Bikoshita Porashar, Pallav Jyoti Arandhara and Anil K Saikia, ***Chem. Commun*. 2021**, *57*, 11701–11704.

Synthesis, Characterization and Properties of Nitrogen Rich Heterocycles: Metal ion Sensors and Transition Metal Chemistry

Dr. V. Manivannan, Ph. D. (IACS, Kolkata)

We are working in the area of "**Synthesis, Characterization and Properties of Nitrogen Rich Heterocycles: Metal ion Sensors and Transition Metal Chemistry**".

Nitrogen rich heterocycles form one of the most important ligands in coordination chemistry. These ligands themselves and/or their metal complexes have versatile applications, *viz.*, DNA binding ability, supramolecular chemistry, enantioselective synthesis, fluorophores, etc. The reactions catalyzed by metal complexes of nitrogen rich heterocycles include oxidation of organic substrates, cleavage of DNA etc., As a part of our programme, we plan to synthesize new substituted nitrogen heterocycles and to investigate their ability as metal ion sensors as well as their coordination chemistry.

Some of the results are published in:

J. Microchem. **2024**, *200*, 110440; ***J. Photochem. Photobiol. A: Chemistry*** **2024**, *450*, 115436; ***J. Photochem. Photobiol. A: Chemistry*** **2023**, *444*, 114913; ***Inorg. Chim. Acta*** **2022**, 535, 120876; ***J. Heterocycl. Chem***. **2022**, 59, 1073–1078; ***J. Photochem. Photobiol. A: Chemistry*** **2022**, *427*, 113795; ***J. Photochem. Photobiol. A: Chemistry*** **2021**, *417*, 113340; ***J. Photochem. Photobiol. A: Chemistry*** **2020**, *394*, 112441; ***Inorg. Chim. Acta*** **2020**, 506, 119506; ***J. Photochem. Photobiol. A*** **2018**, *353*, 77-85; ***ChemistrySelect*** **2017**, *2*, 11727-11731; ***ChemistrySelect*** **2017**, *2*, 11048-11054; ***ChemistrySelect*** **2016**, *1*, 4016-4023; ***Inorg. Chim. Acta*** **2013**, *394*, 210; ***Inorg. Chim. Acta*** **2012**, *390*, 154; ***Tetrahedron*** **2012**, *68*, 3927; ***Tetrahedron Lett.*** **2012**, *53*, 2420; ***Polyhedron*** **2012**, *33*, 9–12; ***Inorg. Chim. Acta*** **2010**, *363*, 1448–1454; ***Tetrahedron Lett.*** **2009**, *50*, 6264–6267; ***Inorg. Chem.*** **2006**, *45*, 7994–7996.

Understanding the Structure-Function Relationship in Supramolecular Chemistry

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Our research group at IIT Guwahati focuses on Supramolecular Chemistry. We explore the use of weak non-covalent interactions to study host-guest chemistry, self-assembly, and crystal engineering. We aim to create intelligent, functional materials by applying the fundamental principles of supramolecular chemistry. Our specific areas of research include Biomineralization and biomimetic material chemistry, Optical sensors for biologically and environmentally essential analytes, Coordination chemistry of cations and anions, Structure-activity relationship of tailor-made (non)-amphiphilic probes, and Environmental chemistry of water treatment.

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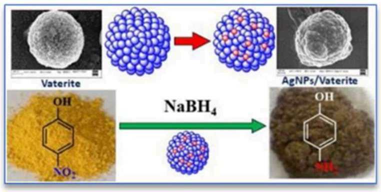
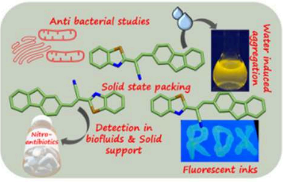
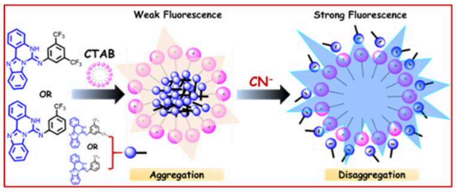
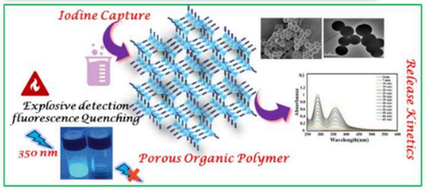
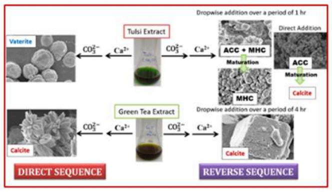
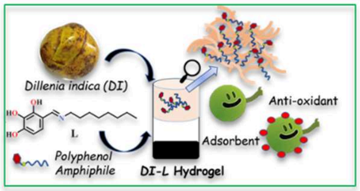












The future direction of our research will be to develop biomimetic materials using the concept of supramolecular chemistry through interdisciplinary research.

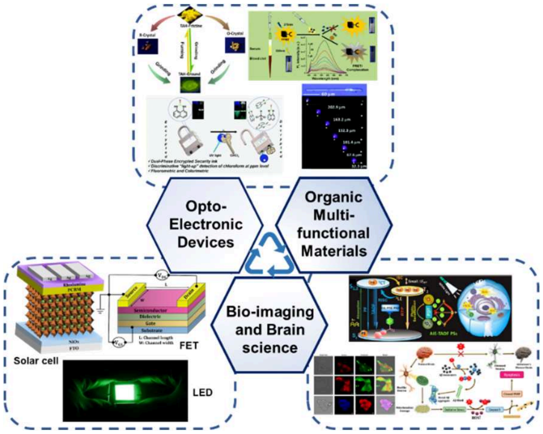
Some of our recent works has been listed below

- Luminogenic and Bactericidal Studies of an Acrylonitrile-based AIEgen. Sagnik De, Debolina Ghosh and Gopal Das, ***Chem. Asian J.*** **2024**, DOI: 10.1002/asia.202400148
- Twisted-Intramolecular-Charge-Transfer Based Fluorogenic Nano-Probe for Ultrafast Cyanide Sensing in Water and Micellar Medium. Oiyao Appun Pegu, Gopal Das, ***J. Mater. Chem. C***, **2024**, DOI:10.1039/D4TC00643G
- Inhibition of Staphylococcal Nuclease by Benzimidazole-based Ligand: Implications in DNA-Mediated Entrapment and Uptake of MRSA by Macrophage-like Cells, Barlina Konwar, Sagnik De, Gopal Das, Aiyagari Ramesh, ***Bioorg. Chem.*** **2024**, DOI:10.1016/j.bioorg.2024.107133
- Dual Functional Porous Organic Polymer: Reversible Iodine Capture and Selective Sensing of Picric Acid, Bikram Mondal and Gopal Das, ***React. Funct, Polym.*** **2024**, DOI:10.1016/j.reactfunctpolym.2023.105800
- Amphiphilic polyphenol incorporated hydrogel derived from mucoadhesive of Dillenia indica: Potential Antioxidant and Adsorbent, Debolina Ghosh, Sagnik De, Deepmoni Deka, Gopal Das, ***Int. J. Biol. Macromol.*** **2024**, DOI: 10.1016/j.ijbiomac.2023.127759
- Anion Induced Intramolecular Cyclisation of Urea-Based Receptors: Entrapment of Cyclic $[SO_4(H_2O)_4{}^{2-}]n$ Cluster and Encapsulation of Anions with varied Dimensionality, Oiyao Appun Pegu, Rubi Moral, Gopal Das, ***Cryst. Growth Des.*** **2023**, DOI:10.1021/acs.cgd.3c01029
- Surfactant Induced Disaggregation of Quinoxaline AIEgen Scaffold: Aggregation Aptitude in Solid and Solution State, Sagnik De and Gopal Das, ***Soft Matter.*** **2023**, DOI: 10.1039/D3SM00638G

Advanced Approaches to Multifunctional Materials

Dr. Parameswar K. Iyer

Over the past few decades, significant advancements have been made in the exploration of organic molecules in multidisciplinary scientific fields. Our mission is to develop new π-conjugated organic molecules (small molecules and polymers) and study their structure and property relationship in detail. These smart functional materials exhibit several advanced photophysical properties like TADF, MR-TADF, RTP, MCL, and NIR, demonstrating excellent performance across various practical applications. These multifunctional materials are utilized to fabricate energy efficient devices for organic light-emitting diodes, photovoltaics, memory devices, thin film transistors, sensory devices, and waveguides. They also find applications in fields like bioimaging, bio-sensor, photodynamic therapy, neurodegenerative disease treatment, and diagnosis, as well as in security information. In addition, the development of new "organic-inorganic" and "biological-synthetic" combination materials is also a focus area of our research. With significant advances in material engineering and device architecture optimization, we have achieved perovskite solar cell efficiency exceeding 22% with stability surpassing 1,000 hours, as well as a maximum luminescence intensity exceeding 25,000 cdm^{-2} in perovskite LEDs. Moreover, the ultra-low operating voltage FET-based biosensor offers rapid & label-free microorganism detection.



Our group aims to contribute to the following societal advancements by the year 2030.

- To explore and understand the mechanistic insights of novel multifunctional materials to enhance their inherent properties for advancement in practical applications.
- To attend exceptionally stable and efficient hybrid halide-based perovskite devices by leveraging multifunctional organic small molecules and polymers as defect passivators for perovskite materials to mitigate their degradation in ambient atmospheres.
- To offer a cost-effective and less intrusive strategy for early diagnosis and treatment of Alzheimer's disease.

1. Barman, D.; Annadhasan, M.; Bidkar, A.; Rajamalli, P.; Barman, D.; Chandrasekar, R.; Ghosh, S. S.; Iyer, P. K.* Highly Efficient Color-Tunable Organic Co-crystals Unveiling Polymorphism, Isomerism, Delayed Fluorescence for Optical Waveguides and Cell-imaging ***Nat. Commun.*** **2023**, *14,* 6648.
2. Barman, D.; Annadhasan, M.; Chandrasekar, R.*; Iyer, P. K.* Hot-Excitons Harvesting via Through-Space Single-Molecule Based White-Light Emission and Optical Waveguides. ***Chem. Sci.*** **2022**, *13*, 10224-10254.
3. Ghosh, P.; Shokeen, K.; Mondal, S.; Kandasamy, T.; Kumar, S.; Ghosh, S. S.; Iyer, P. K.* Amyloid Targeting Red Emitting AIE Dots for Diagnostic and Therapeutic Application against Alzheimer's Disease. ***ACS Chem. Neurosci.*** **2024**, *15*, 268-277.
4. Gupta, R. K.; Garai, R.; Iyer, P. K.* Trap State Passivation for Stabilizing Perovskite Solar Cells via Multifunctional Molecules. ***Acc. Mater. Res.*** **2023**, *4*, 560-565.
5. Garai, R.; Gupta, R.K.; Hossain, M.; Iyer, P. K.* Surface recrystallized stable 2D-3D graded perovskite solar cells for efficiency beyond 21%. ***J. Mater. Chem. A,*** **2021**, 9, 26069-26076.

Resonance: Electron-molecule scattering in atoms and molecules

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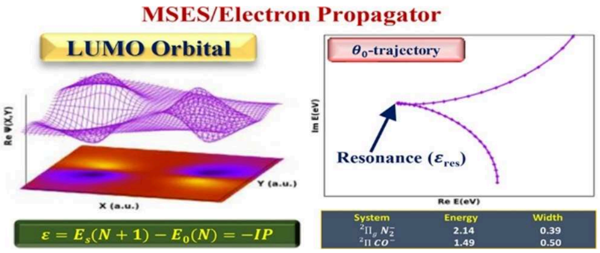
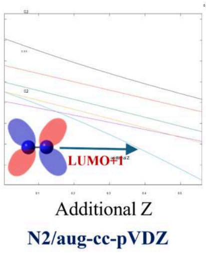
We are interested in studying resonance or metastable states in atoms and molecules. Resonances are one of the most important phenomena in electron-molecule scattering. These are exponentially decaying long-lived metastable states of a system. These metastable states with a finite lifetime can break up into twoor more subsystems. These states can be considered as discrete states that are coupled to the continuum. The resonance energies are represented by the complex energy equation$E = E_r - \frac{i\Gamma}{2}$, where E_r and Γ are the energy position and the width of the resonant states, respectively. These complex energies can be obtainedby imposing purely outgoing boundary conditions on the wave functions of the time-independent non-Hermitian Hamiltonian. The associated wave functions also do not correspond to the Hermitian domain of the Hamiltonian and, hence, are not square integrable. The method of analytical continuation of the Hamiltonian can be performed inthe complex plane to make the resonance function square integrable. The complex scaling (CS) method and complex absorbing potential (CAP) method are the most extensively used techniques in this case. In our group, we have developed a modified smooth exterior scaling (MSES) method to expose the resonance. The MSES method is an efficient method to impose outgoing boundary conditions in electron–atom or electron–molecule scatterings. MSES can be used to convert divergent wave functions to square integrableones.

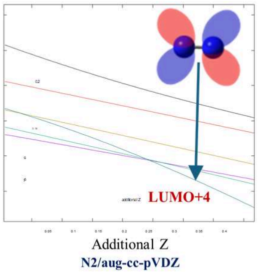
We are further interested in the identification of the Lowest Unoccupied Molecular Orbital (LUMO) which is very essential in studying the resonance phenomenon. In molecules, defining virtual orbitals obtained from SCF calculation is not straightforward and depends heavily on the basis sets used. For instance, when using a highly diffused basis set, the energy for the lowest empty molecular orbital (MO) will be almost zero, making it unreliable. We have developed an innovative approach using parametric equations of motion (PEM) in conjunction with the nuclear charge stabilization method to identify the LUMO obtained from the SCF solution exhibiting stability with different basis sets, including diffused functions.



$\varepsilon = E_s(N+1) - E_0(N) = -IP$

System	Energy	Width
$^2\Pi_g$ N_2^-	2.14	0.39
$^2\Pi$ CO^-	1.49	0.50





References

1. Banuary, M.; Gupta, A. K. Application of Modified Smooth Exterior Scaling Method to Study $^2\Pi_g$ N_2^- and $^2\Pi$ CO^- Shape Resonances. ***ACS omega* 2023**, 8, 7143–7150.

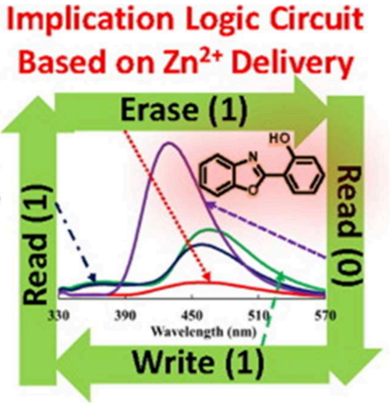
2. Banuary, M.; Kumar, D.; Gupta, A. K. Use of the dilated electron propagator in conjunction with themodified smooth exterior scaling method to characterize ^2S Be$^+$(1s^{-1}), ^2S Ne$^+$(1s^{-1}) Auger and ^2P Be$^-$ shape resonances. ***New J. Chem.* 2024**, 48, 4772–4782.

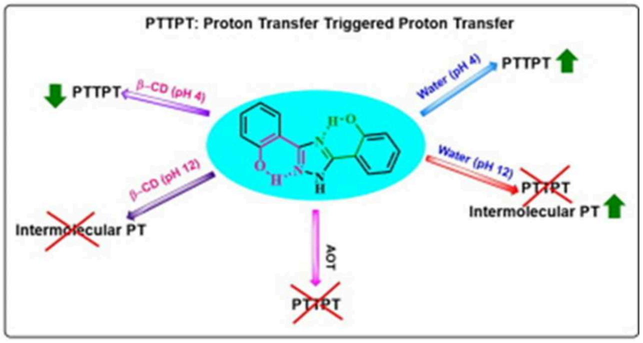
3. Kalita, D. J.; Gupta, A. K. Use of modified smooth exterior scaling method as an absorbing potentialand its application. ***J. Chem. Phys.* 2011**, 134.

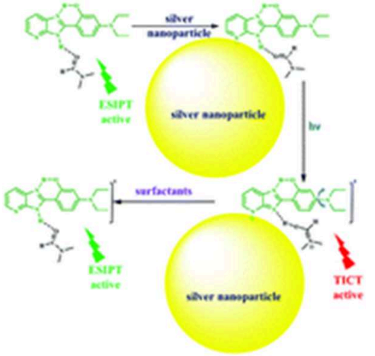
Understanding the mechanism of multiple luminescence and developing molecules for sensing and other applications

Dr. G. Krishnamoorthy

Our group is interested in investigating the different mechanisms of photophysical processes. We are also interested in developing molecules for sensing and other applications. Molecules which emit multiple luminescence have the advantage to use as ratiometric sensors. This property makes them qualify as concentration-independent sensors. The mechanisms for such emissions are also of interest. Photophysical processes such as excited state intramolecular proton transfer (ESIPT) and intramolecular charge transfer (ICT) often result in dual or multiple emissions; therefore, we investigated those processes with special attention.







Few publications:

1. Excited state dynamics of a double ESIPT unit comprising fluorophore, ***J. Photochem. Photobiol. A: Chem***., **2024**, 450, 115412.
2. Role of explicit hydrogen bonding in solvation calculation on the photophysics of 2-(2'-hydroxyphenyl)oxazolo [4, 5-b] pyridine, ***J. Mol. Liq***. **2024**, 394, 123765.
3. Host-guest interaction aided Zinc carry and delivery by ESIPT active 2-(2'-hydroxyphenyl) benzoxazole, ***Spectrochim Acta A Mol Biomol Spectrosc***., **2022**, 281, 121474.
4. Nanoparticle and surfactant controlled switching between proton transfer and charge transfer reaction coordinates, ***Phys. Chem. Chem. Phys***, **2022**, 24 (8), 4944-4956.
5. Light-driven switching between intramolecular proton-transfer and charge-transfer states, ***J. Phys. Chem., B*** **2021**, 125 (9), 2339-2350.

NO Chemistry Laboratory

Dr. Biplab Mondal
https://fac.iitg.ac.in/biplab/index.html

Currently, we have been involved in studying the transition metal complexes -HNO/NO- chemistry. HNO is known to react with metalloproteins, thiols, and there is a significant overlap of its reactivity with NO. For instance, HNO and NO, both are reactive towards heme-proteins in both the FeII and FeIII states. However, the examples of HNO/NO^- donors still remain restricted to only a few such as Angeli's salt, Piloty's acid or acyl and acyloxy nitroso derivatives; but, all of these have some intrinsic limitations like the simultaneous release of undesirable byproducts, ineffective release of HNO at physiological pH etc. Hence, there is a need for more efficient HNO donors.

The metal bound nitrosyl complexes with suitable electronic configurations have been found to be efficient HNO donors. Our lab is actively engaged in developing metal nitrosyl complex based HNO/NO-donors.

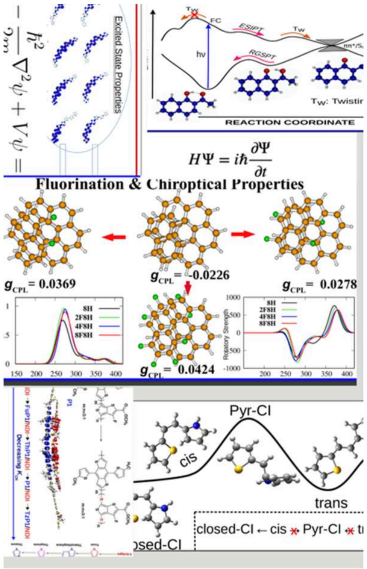
We are also exploring the small molecule models for reductase enzymes which catalyzes the reduction of nitrite to nitric oxide or nitrous oxides as well the activation of nitric oxide using transition metal complexes.

For further details:

1. Saha, S.; Maity, S.; Mazumdar, R.; Samanta, B.; Ghosh, R.; Guha, A.; Mondal, B. ***Inorg. Chem***., **2023**, 62, 17074.
2. Samanta, B.; Ghosh, R.; Mazumdar, R.; Saha, S.; Maity, S.; Mondal, B. ***Dalton Trans***., **2023**, 52, 15815.
3. Mazumdar, R.; Saha, S.; Samanta, B.; Ghosh, R.; Maity, S.; Mondal, B. ***Dalton Trans***., **2023**, 52, 7917.
4. Mazumdar, R.; Mondal, B.; Saha, S.; Samanta, B.; Mondal, B. ***J. Inorg. Biochem***., **2022**, 228, 111698.
5. Mazumdar, R.; Saha, S.; Samanta, B.; Mondal, B. ***Inorg. Chem***., **2021**, 60, 18024.

Computational and Theoretical Chemistry Laboratory

Dr. Aditya N. Panda



Understanding chemical and physical processes at the molecular level is of paramount importance as this seeks to answer what happens when a chemical or physical process occurs. In recent times, our computational group has been involved in modeling the processes involved in organic solar cells and organic light-emitting diodes. Static studies at the molecular level have highlighted the importance of halogen atom substitution and π bridges on donor-acceptor-based systems. In addition, we have also been exploring diverse types of modifications in helicenes to explore their chiroptical properties. Helicenes are inherently chiral, and these are of fundamental importance in various applications such as in asymmetric catalysis, fluorescent sensors, and quantum computers. On another front, semiclassical non-adiabatic dynamics studies have also been carried out to understand the photophysics in ESIPT-based systems. Recently, we have started exploring the oligomers of pyridine and pyrdine-like systems to understand their structure and properties in the excited states.

In the future, we plan to take the above studies forward to develop and implement methods to study the dynamics in excited states. As these systems are quite large, we will develop reduced-dimensional quantum mechanical models to study quantum dynamics. In addition, semiclassical on-the-fly methods will also be used to check their applicability to understand the dynamics happening at the donor-acceptor interfaces, in helicenes, and in oligomers of various systems. We also aim to apply machine learning in the above-mentioned dynamical studies.

1. Mohd Shavez and Aditya N. Panda, Assessing Effects of Different π bridges on Properties of Random Benzodithiophene-thienothiophene Donor and Non-fullerene Acceptor Based Active Layer, ***J. Phys. Chem. A,*** **2021**, 125, 9852
2. Bishwanath Mahato and Aditya N. Panda, Effects of Heterocyclic Ring Fusion and Chain Elongation on Chiroptical Properties of Polyaza[9]helicene: A Computational Study, ***J. Phys. Chem. A***, **2022**, 126, 1412.
3. Ibanrishisha Mawa and Aditya N. Panda, Insights into the Excited-State Processes in 1-Hydroxy-2-acetonaphthone at ADC(2) and CASSCF Levels, ***J. Phys. Chem. A,*** **2021**, 125, 3015.
4. Bishwanath Mahato and Aditya N. Panda, Effect of Terminal Fluorination on Chiroptical Properties of Carbo[5−8]helicenes: A Systematic Computational Study at the RI-ADC(2) Level ***J. Phys. Chem.*** *A* **2023**, 127, 2284.
5. Ibanrishisha Mawa and Aditya N. Panda. Theoretical Investigation of the E/Z Photoisomerization Pathway in 1-(2-Pyrrolyl)-2-(2-thienyl)ethylene, ***J. Phys. Chem. A*** **2023**, 127, 5673.
6. Palak Mandal and Aditya N. Panda, Conformational Effect on the Excitonic States of 2-Phenylpyridine Oligomers: Ab Initio Studies and Analysis, ***J. Phys. Chem. A*** **2023**, 127, 7898.

Computational Chemistry and Biophysics Lab

Dr. Sandip Paul

Email: sandipp@iitg.ac.in
Group Website: https://sandipp8.wixsite.com/sandippaul

Our research is dedicated to advancing the field of Computational Biophysics and Chemistry, with a particular emphasis on small molecules, peptides, and proteins. Our group is committed to uncovering new insights that will shape the future of scientific discovery and innovation. We use Classical Molecular Dynamics Simulation, Replica Exchange Molecular Dynamics (REMD), Markov State Modelling, Machine Learning, Quantum Mechanics/Molecular Mechanics (QM/MM) and Umbrella Sampling Technique as tools in our study. Our current and visionary projects for 2030 span these domains:

⇒ **Tweezer molecules** can bind to diverse substrates owing to their exquisite flexibility. We are exploring their potential uses in complex topological systems, protein inhibition, and modulation of G protein-coupled receptors (GPCRs).

⇒ **Antimicrobial peptides** are the body's primary defence against pathogens. We are investigating their conformational dynamics, aggregation pathways, and membrane permeabilization properties, as well as their potential therapeutic uses.

⇒ **Cyclic peptides** self-assemble in water to form nanotube-like structures. We are studying the behaviour of cyclic peptides across different physical environments and to explore their possible applications as drug delivery agents and transport channels.

⇒ The presence of **knots in proteins** is an enigma that can hinder their folding efficiency when compared to unknotted proteins. Despite this, they exist in a variety of proteins. We are studying the conformational dynamics and functionalities that knots impart to the parent proteins.

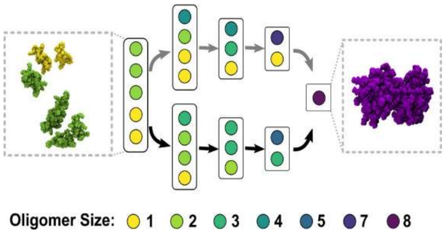
⇒ Peptide aggregation leads to severe diseases in the human body. Among all aggregating peptides, the **human calcitonin (hCT)** peptide is responsible for medullary carcinoma of the thyroid gland. We are inhibiting the aggregated hcT peptides with a varied class of inhibitors.

⇒ **Glycolytic enzymes** play a crucial role in cellular glucose metabolism. We are investigating the structural dynamics of their active site conformers and their effects towards substrate binding.

⇒ **Conotoxins**, a class of neurotoxic peptides found in the venom of cone snails, have gained importance due to their selectivity and potency as drugs. We are focusing on the various classes of conotoxins and studying their interactions with target receptors.

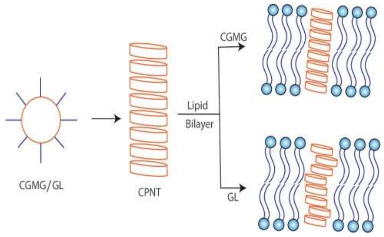
Our recent works

Pathways of oligomerization in hIl-37$_{17-29}$



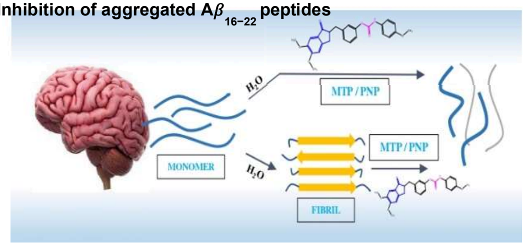
Mitra, A.; Paul, S. Pathways of hIl-3717-29 Aggregation Gives Insight into the Mechanism of α-Amyloid Formation. ***J. Phys. Chem. B* 2023,** 127, 8162–8175, DOI: 10.1021/acs.jpcb.3c04742

Insertion of CPNT across bilayers



Moral, R; Paul, S. Exploring Cyclic Peptide Nanotube Stability Across Diverse Lipid Bilayers and Unveiling Water Transport Dynamics. ***Langmuir* 2024**, 40, 882-895, DOI: 10.1021/acs.langmuir.3c03030.

Inhibition of aggregated Aβ_{16-22} peptides



Paul, R; Sawoo, D; Devi, M; Paul, S. Inhibitory Action of Indanone-Carbamate Hybrid Molecules on the Aggregation of Aβ_{16-22} Peptides and Their Translocation across POPC Lipid Bilayer. ***J. Mol. Liq.* 2023**, 383, 122028-122042, DOI: 10.1016/j.mollliq.2023.122028

Designing energy storage systems through diffusion control

Dr. Mohammad Qureshi

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Energy storage based on its applications is a smart approach in today's scenario. Battery technology is continuously thriving with new molecules on horizon for improved energy density and volumetric storage. However, some modern transport and energy storage applications need power density as the essential component along with the reasonable, if not battery like energy storage. This scenario emerges into designing supercapacitor based batteries or we call Super Batteries. Supercapacitor energy storage dominantly depend on electric charge storage via double layer formation, where as conventional battery energy storage depends on Faradic reactions. Our approach is to design materials and fabricate devices to balance between EDLC and Faradic process to achieve better energy density than conventional super capacitors and better power density than conventional batteries. In addition, we have shown the external and internal stimuli can have their dominant effect in deciding energy storage mechanism and thereby their outcomes.

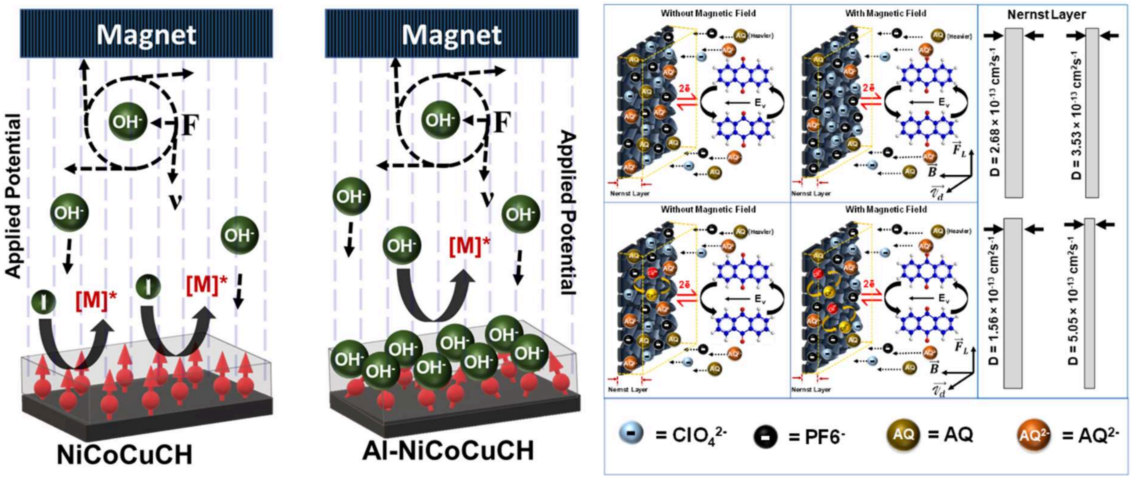


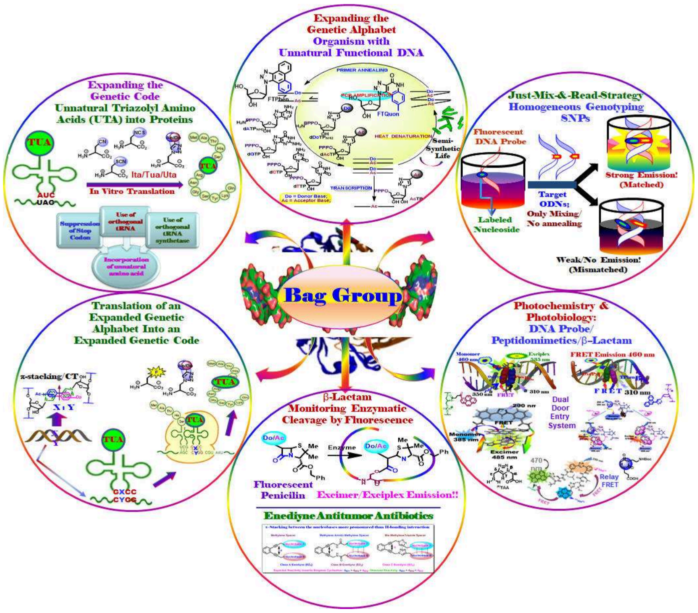
Figure 1: (Left) Effect of external magnetic field on diffusional controlled energy storage (Right) Use of non-magnetic ions under the external magnetic field and their influence on diffusion characteristics

References: (1). Alpana Sahu, Peeyush Pandey, Sourav Bhowmick, and Mohammad Qureshi, ***Chem. Commun***., **2023,** 59, 1038; (2) Peeyush Pandey, Sourav Bhowmick, Mohammad Qureshi, ***ACS Appl. Mater. Interfaces* 2023,** 15, 39435, (3) Anjana Singh, Peeyush Pandey, Alpana Sahu, and Mohammad Qureshi, ***J. Phys. Chem. Lett.* 2024**,15, 2123.

The Bag Laboratory

Dr. Subhendu Shekhar Bag

The Vision 2030 of Prof. Bag's research group, located at the Department of Chemistry, IIT Guwahati, is a pioneering blueprint aimed at pushing the frontiers of synthetic biology, personalized medicine, and nanotechnology. At the core of their vision is the creation of a semi-synthetic organism through the groundbreaking fields of genetic alphabet and genetic code expansion. By incorporating unnatural base pairs and expanding the genetic code by incorporating unnatural amino acids with tailored properties, the group aspires to develop novel biological systems with extraordinary capabilities. Further, in personalized medicine, the group is committed to advancing genotyping technologies for Single Nucleotide Polymorphisms (SNPs). This effort is crucial for tailoring medical treatments to individual genetic profiles, ultimately improving therapeutic outcomes and reducing adverse effects. Concurrently, the group is innovating in the design of fluorescent β-lactam antibiotics, aiming to revolutionize the detection and treatment of bacterial infections with greater precision and efficacy.



Additionally, the group's research on radical generating hybrid organics, such as enediyne - nucleoside / peptide conjugates, has the potential to produce highly effective anticancer agents, offering new hope in the fight against cancer, which is a growing burden in India. Furthermore, our innovations in biosensor and chemical sensor development for the fluorescent detection of beta-lactamases and label-free DNA detection are set to revolutionize diagnostic techniques, leading to earlier and more accurate disease detection and management. Moreover, in synthetic methodology, the group is pioneering new chemical reactions, including Click-Sonogashira Coupling, One Pot Click and Sonogashira, and the use of unnatural amino acid atrop-isomers as catalysts for asymmetric synthesis and organic photocatalysis. These innovations are expected to streamline complex synthetic processes, making them more efficient and sustainable. Finally, the group's exploration into nano-biomaterials and nano-photocatalysis is set to address critical issues in healthcare and environmental sustainability. The development of biomaterials for burn wound healing has significant implications for defence applications, while their photocatalytic approach to treating hospital and community-generated wastewater represents a crucial step towards mitigating environmental pollution.

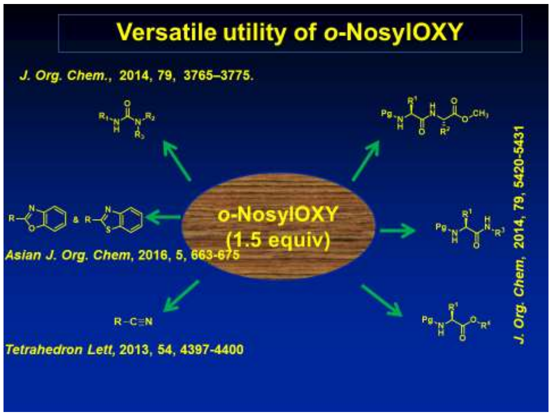
Overall, Prof. Bag's visionary research aligns with India's scientific and socio-economic goals, fostering innovation that promises to drive progress across healthcare, industry, and environmental sustainability.

Laboratory of Peptide and Amyloid Research

Dr. Bhubaneswar Mandal

What we have achieved so far:

- Our versatile recyclable coupling reagents for waste reduction in pharmaceutical industries: Boc-Oxyma (CAS No. 1426821-11-5), ortho-NosylOXY (CAS No. 1441409-96-6), para-NosylOXY (CAS No. 1441409-91-1).



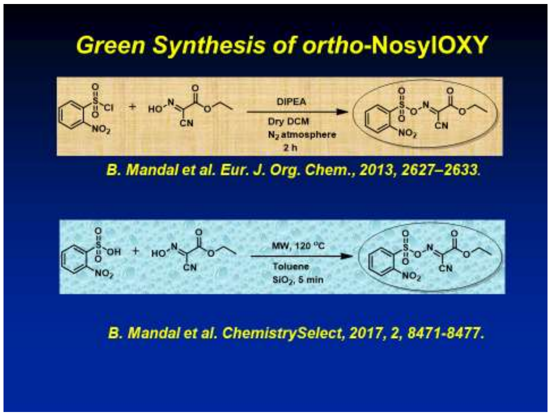
Versatile utility of *o*-NosylOXY

J. Org. Chem., 2014, 79, 3765–3775.

Asian J. Org. Chem, 2016, 5, 663-675

Tetrahedron Lett, 2013, 54, 4397-4400

J. Org. Chem, 2014, 79, 5420-5431

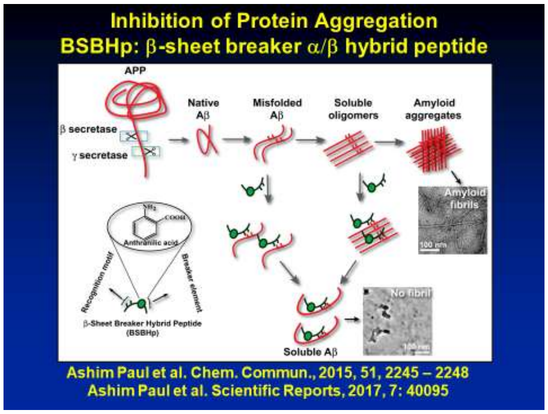


Green Synthesis of ortho-NosylOXY

B. Mandal et al. Eur. J. Org. Chem., 2013, 2627–2633.

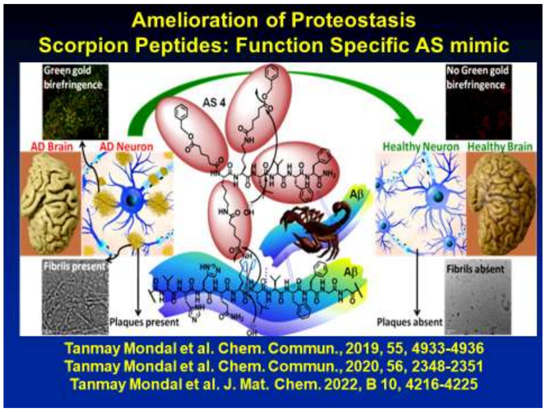
B. Mandal et al. ChemistrySelect, 2017, 2, 8471-8477.

- Development of a few new drug design strategies for amyloid diseases.



Inhibition of Protein Aggregation
BSBHp: β-sheet breaker α/β hybrid peptide

Ashim Paul et al. Chem. Commun., 2015, 51, 2245 – 2248
Ashim Paul et al. Scientific Reports, 2017, 7: 40095



Amelioration of Proteostasis
Scorpion Peptides: Function Specific AS mimic

Tanmay Mondal et al. Chem. Commun., 2019, 55, 4933-4936
Tanmay Mondal et al. Chem. Commun., 2020, 56, 2348-2351
Tanmay Mondal et al. J. Mat. Chem. 2022, B 10, 4216-4225

What want to achieve by 2030:

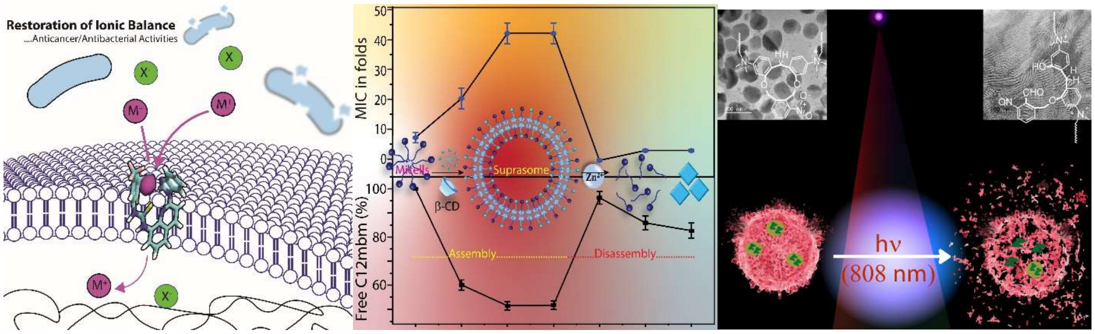
- Development of new strategies for sustainable industrial practice.
- Development of artificial proteasome as a new drug design strategy for amyloidosis.

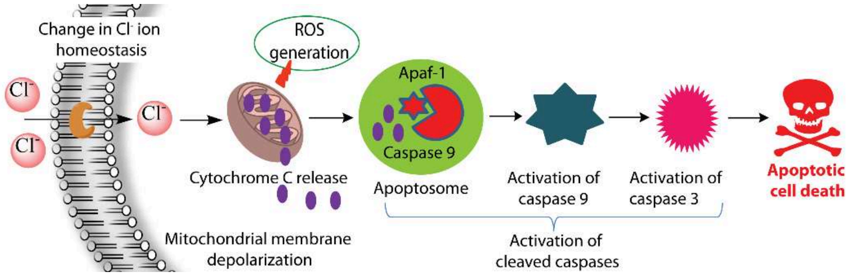
Biological Chemistry Laboratory

Dr. Debasis Manna, Ph.D.

Email: dmanna@iitg.ac.in
Website: https://fac.iitg.ac.in/dmanna/Home.html

We are a group of researchers working in the areas of biological chemistry, organic chemistry and physical chemistry. We are involved in integrating the concepts and approaches from synthetic chemistry and physical chemistry to apply in chemical biology. We design and synthesize lipophilic organic molecules for ion recognition, transmembrane ion transport, chemical biology and other fields. We are also interested in developing drug delivery systems to deliver specific drugs (antibacterial or anticancer agents) and synthetic ion transporters to the cells (bacterial or mammalian) for diverse applications in chemistry and biology.





Recent Publications

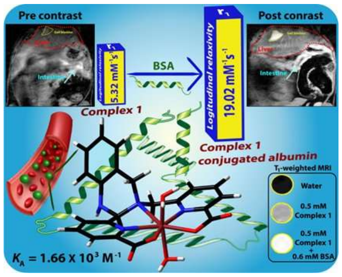
1. Dey, S., Patel, A., Haloi, N., Srimayee, S., Paul, S., Barik, G. K., Akhtar, N., Shaw, D., Hazarika, G., Prusty, B. M., Kumar, M., Santra, M. K., Tajkhorshid, E.*, Bhattacharjee, S.*, and Manna, D.* ***J. Med. Chem.*, 2023**, 66, 11078-110932.
2. Prusty, B. M., Karn, R., Patel, A., Mazumder, P., Kumar, S., Manna, D* ***Chem. Commun.***, **2023**, 59, 10624-10627.
3. Dey, S.; Chatterjee, S.; Patel, A.; Pradhan, N.; Srivastava, D.; Patra, N.; Bhattacharyya, A.; Manna, D.* ***Chem. Commun.***, **2021**, 57, 4646-4649.
4. Akhtar, N.; Biswas, O.; Manna, D.* ***Chem. Commun.***, **2020**, 56, 14137-14153.

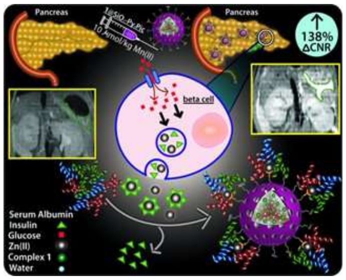
Dr. Chandan Mukherjee

Ph.D.	Max-Planck Institute for Bioinorganic Chemistry Muelheim an der Ruhr, Germany (2003-2006)
Postdoc	Bielefeld University, Germany (2007-2010)
Postdoc	The University of Tokyo, Japan (2010-2011)
Professor	Indian Institute of Technology, Guwahati (since 2019)

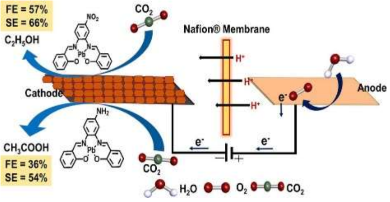
Our research group focuses on developing inorganic metal complexes and redox-active organic molecules aiming the understanding of fundamental properties and applicability towards the emergence of new: (i) MRI contrast reagents (MRI-CAs), (ii) catholytes and anolytes for redox-flow non-aqueous batteries, (iii) catalysts for the generation of fuels from H_2O/ CO_2 /N_2, and (iv) semiconductors for the application in spintronics: materials for artificial intelligence and neuromorphic computation.

For the development of new MRI contrast agents; we have chosen nutritional Mn(II) and Fe(III) metal ions to instate the biogenic properties in the metal complexes formed by the coordination of the ions with water-soluble organic molecules (ligands). To enhance the effectiveness of the CAs, our group has initiated a unique modification where the complex molecules are confined within a porous silica nanoparticle. Further, we have achieved organ and functional-specific MRI-CAs by clubbing the surface of the silica nanosphere with suitable organic molecules, *e.g.*, folic acid, *ortho*-methoxybenzene, bis(picolinic acid), etc.

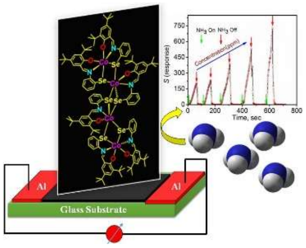




Carcinoma is a lethal disease, and day by day, the number of patients with the disease is increasing. An early-stage detection of carcinoma will increase survival chances. In this regard, we are currently focusing on engendering MRI-CAs for very early-stage cancer detection. Additionally, we are concentrating on materializing ATP-sensitive MRI-CAs. The rate of cell division in the ovary and testes is the highest in the human body, and ATP is essential for this purpose. Furthermore, the development and function of granulosa and theca cells (constitutes of an ovarian follicle) are driven by ATP. Therefore, ATP-sensitive MRI-CAs will be immensely important for diagnosing human reproduction systems *via* MR images. We have successfully engendered some metal complexes as catalysts to study the electrochemical reduction of CO_2 to carbonaceous fuels and various feedstocks for chemical industries. However, the higher overpotential initiates hydrogen production and affects selectivity.



In the future, we will focus on developing ligand-based radical-containing metal complexes, which will minimize the overpotential and elevate the product-selectivity and stability of the catalysts as the oxidation state of the metal ions will remain intact and ligand-based redox activity, which occurs at a much lower potential, will be functional in the catalytic conversion.



We are motivated to comprehend the electronic properties of radical-containing transition complexes for the possible application as semiconductors, which have immense use in materializing data storage materials, supercapacitors, sensors, and spin filters. In this context, some polynuclear transition metal complexes and organic compounds have already been examined and found to be effective for (i) sensing ammonia gas, (ii) developing hardware for neuromorphic computation and software as well as hardware for artificial intelligence, and (iii) realizing electrochromic materials. In the coming days, we shall continue in these endeavors.

Molecules to Materials: Journey Through Self-Assembly Route

Dr. A. S. Achalkumar

PhD: Centre for Nano and Soft Matter Research, Bangalore (2007)
Postdoc: Centre for Molecular Nanoscience (CMNS, University of Leeds,
Leeds, UK (2009); RIKEN Advanced Science Institute,
Wakoshi, Saitama, Japan (2011)
Professor: Department of Chemistry (2019 onwards), IIT Guwahati
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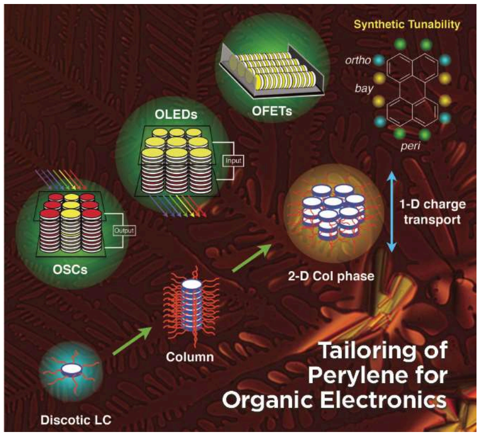
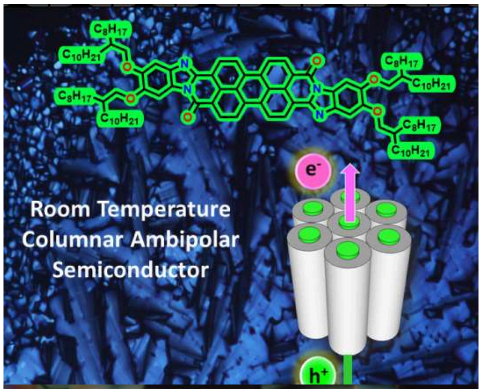
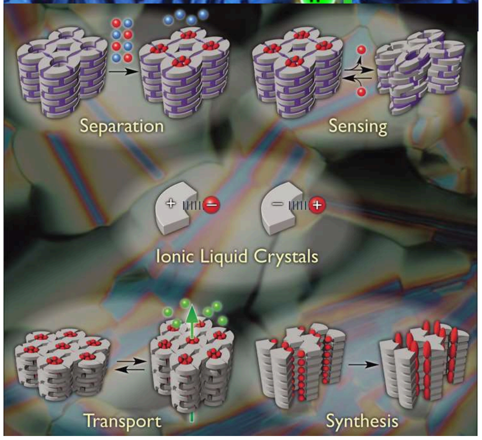
Liquid crystals (LCs) are often termed as fourth state of matter and they are ubiquitous in nature. LC self-assembly, often unraveled the mysteries of complex systems such as solid crystals and living systems. They are also sensitive to several kinds of external stimuli, which can be exploited towards applications.

- We are interested in the molecular design and synthesis of discotic liquid crystals (DLCs), which can self-assemble into technologically important nematic (N) and columnar (Col) phases. Nematic phase of DLCs is known to reduce the wide viewing angle problem of twisted nematic liquid crystal displays (TNLCDs), whereas a well-aligned Col phase can revolutionize the existing organic photovoltaics (OPVs), field effect transistors (FETs), organic light emitting diodes (OLEDs) and gas sensors due to its one-dimensional charge carrier mobility.
- LCs as organized fluids can be versatile chiral reaction media, while their polymerized frameworks have a great potential in chiral separation. We also want to explore lyotropic liquid crystals as biomembrane mimics, because these investigations can have far reaching impacts on the biological and medicinal fields.
- In addition, we would like to design and synthesize several stimuli responsive functional molecules and engineered surfaces that will have applications in in analytical chemistry, catalysis, electronics, molecular recognition and nanotechnology related fields.
- Further there will be increased efforts to integrate different properties in a single molecule, so as to simplify the device structure, minimize the expenses without compromising the efficiencies. In a nutshell, we want to explore different realms of supramolecular self-assembly and functional materials through the power of Organic Chemistry.



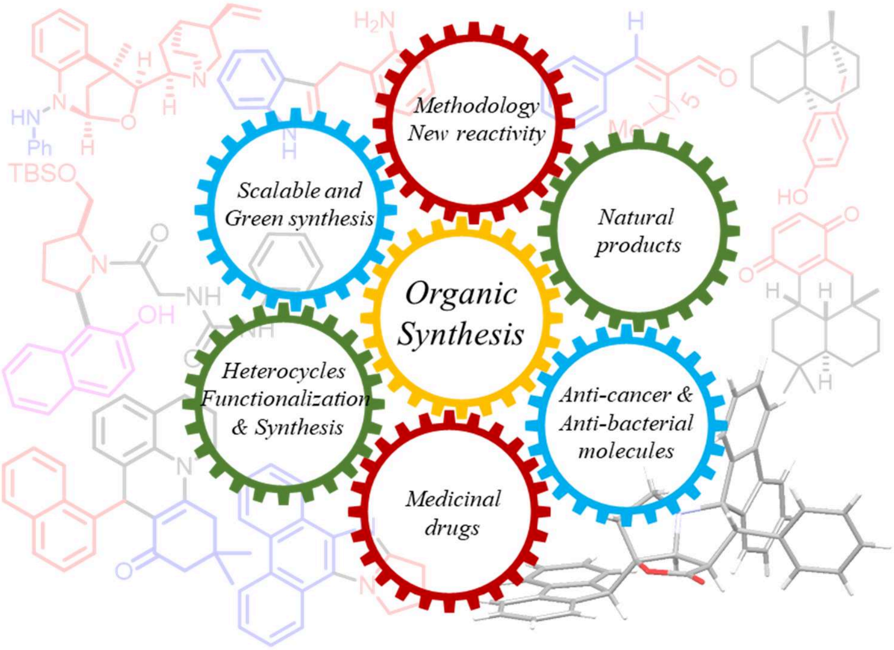




Dr. Chandan K. Jana

Functional organic molecules serving as medicinal drugs are continuing to have a tremendous impact on modern society. The innovative design of such novel molecular entities such as natural products and their unnatural derivatives, bioactive heterocycles, etc., the development of their scalable and green synthetic routes, and studies of their functional properties to identify the most potent candidate are the prime goals of our research.

Our research contributed significantly to different areas such as green chemistry, carbon-hydrogen bond functionalization, heterocyclic chemistry, catalysis, and synthesis of natural products and their unnatural derivatives in the field of chemical science. In the context of the medicinal value of organic molecules, the research group could synthesize and identify new synthetic terpenoids and heterocyclic compounds possessing excellent anti-bacterial and anti-cancer activities with micro-to-nano-molar IC_{50} concentrations.



Our research program will continue developing new reactivity/methods, scalable and green synthetic strategies that will enrich the field of organic chemistry as well as provide means to affordable source to value-added chemicals, pharmaceuticals, organic materials, etc. Taking our lead bioactive molecules, we also aim to develop new therapeutic agents against cancer and multi-drug-resistant bacteria.

Supramolecular Chemistry Lab

Dr. Debapratim Das

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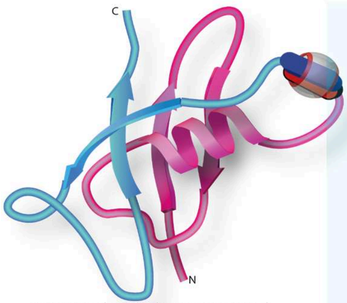
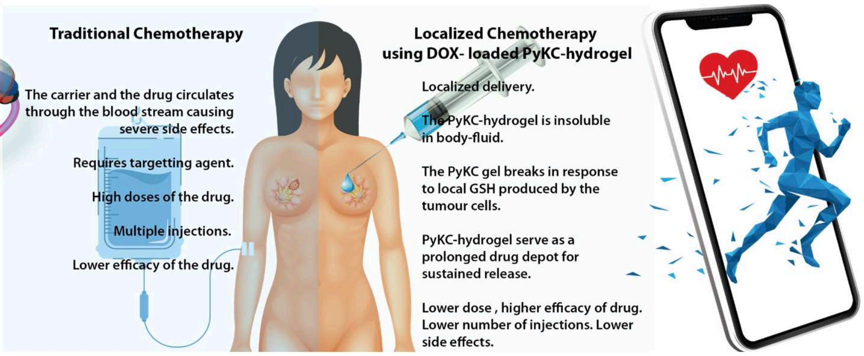
In the supramolecular chemistry lab, we work on various aspects of supramolecular soft materials. Part of our endeavors is directed at understanding supramolecular interactions and host-guest complexation, especially with Cucurbiturils. Other aspects of our research focus on the preparation of soft materials for biomedical and other applications. Below is the bucket list of our wishes that we want to achieve by 2030.

- Peptide-hydrogel-based localized drug delivery systems to cure breast and kidney cancer. The system will be GSH-responsive and will deliver the drug in response to the excess GSH present at the tumor.
- We aim to prepare soft-micro beads using peptide-based hydrogels. Eventually, we aim to create point-of-care diagnostic devices using these microbeads.
- Recently, we started working on "Systems Chemistry," and we are developing transient assemblies. Our aim is to achieve transient systems that can generate a wide spectrum of light, and the light will be utilized for photocatalysis in a transient manner.
- In recent years, we started working on polymeric soft gels and we aim to create new and efficient motion sensors and fire-retardant paints using these materials.
- Last but not least, our dream project is to create a fully functional protein/enzyme from its peptide fragments using the ternary complexation by Cucurbit[8]uril. We are hopeful to achieve this new "split protein" technique that will open up many future prospects in this area.



Supramolecularly regenerated functional Ubiquitin



References:

1. ***Angew. Chem. Int. Ed.* 2024** (https://doi.org/10.1002/anie.202414239).
2. ***ACS Appl. Mater. Interfaces* 2024**, *16*, 5183–5195.
3. ***Chem. Eng. J.* 2023**, *477*, 147105.
4. ***Adv. Optical. Mater*. 2023**, 2301422.
5. ***Chem. Sci.* 2022**, *13*, 4050-4057.

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Numerous aspects of chemistry impact our lives. It enhances our well-being by creating medications to cure illnesses. Making the correct enantiomer of a medicinal molecule can be the difference between life and death. Patients with Parkinson's disease are treated with Dopa, a non-proteinogenic α-amino acid. Dopa is chiral, and its only useful form for regaining nerve function is (S)-Dopa.[1] (R)-Dopa is highly poisonous in addition to being ineffectual. Therefore, only one enantiomer of the medication may be delivered. This is just one instance of many where the enantiomeric versions of a given chemical cause distinct reactions in biological systems.

Potency, selectivity, and desirable physical qualities are required for possible therapies to have molecular complexity with one or more asymmetric centers because to the ever-increasing problems in treating both novel and established diseases. To achieve the necessary physical, chemical, and biological properties, molecules must be prepared in enantiomerically pure forms.

The pharmaceutical sector will need to lower its pricing because many countries will not be able to pay the treatments for chronic diseases like diabetes, even though their social and economic value will increase in the future years. Chemists must discover quick, easy, and widely applicable methods for creating novel drug candidates for testing in small-scale laboratory synthesis before they can proceed to such a low-cost, successful commercial manufacturing. Creating atom-efficient, single-pot, multi-component, catalytic (asymmetric) reactions is one way to tackle this problem.[2]

In the upcoming years, we hope to create atom-economic, one-pot, catalytic asymmetric processes with organic or organometallic catalysts. Benjamin List and David MacMillan are awarded the Nobel Prize in Chemistry 2021 for their development of a new and ingenious tool for molecule building: organocatalysis.[3,4] Recently, our group got interested in sequential catalysis and dearomatization reactions.[5,6]

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1. P. Warot, *Lille médical: journal de la Faculté de médecine et de pharmacie de l'Université de Lille* **1971**, *17*, 329-334.
2. I. Ojima, in *Catalytic Asymmetric Synthesis,* Wiley-VCH, Weinheim, **2008**.
3. D. W. C. MacMillan*, The advent and development of organocatalysis,* ***Nature***, **2008***, 455,* 304-308.
4. S. C. Pan, B. List, *New Concepts for Organocatalysis*, in *Organocatalysis* (M. Reetz, B. List, S. Jaroch, H. Weinmann (Eds.), Springer **2008,** 1-45.
5. R, Khuntia, S. K. Mahapatra, L. Roy, S. C. Pan, *Structurally divergent enantioselective synthesis of benzofuran fused azocine derivatives and spiro-cyclopentanone benzofurans enabled by sequential catalysis,* ***Chem. Sci.*** **2023**, *14*, 10768-10776.
6. A. Shikari, C. Parida, S. C. Pan, *Catalytic Asymmetric Dearomatization of 2,3-Disubstituted Indoles by a [4 + 2] Cycloaddition Reaction within Situ Generated Vinylidene ortho-Quinone Methides: Access to Polycyclic Fused Indolines*, ***Org. Lett.*** **2024**, *early view* https://doi.org/10.1021/acs.orglett.4c00557

Laboratory of Biomolecules

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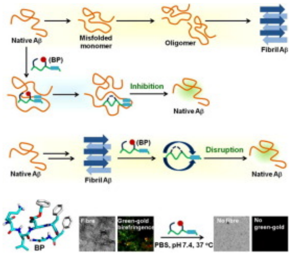
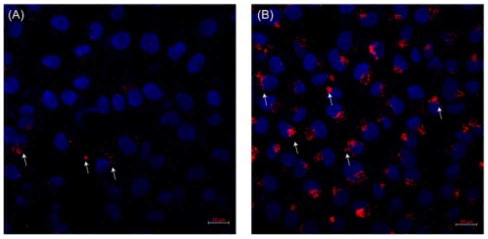
The chemistry of biological macromolecules such as DNA, proteins, and carbohydrates and small molecules such as vitamins, fatty acids, and cholesterol are extremely fascinating to understand and regulate their biological functions in living cells. Life-threatening diseases, including tumor growth and Alzheimer's, occur due to the malfunctions of the chemistry of the biomolecules. Tunable, chemically altered biomolecules are often used as molecular probes to study chemistry inside cells. Moreover, chemically modified biomolecules with improved physiological properties can be formulated into nanomaterials for effective, target-specific delivery of small molecules.

The present focus of our laboratory is to develop synthetic, designer peptides that undergo *in-situ* self-cyclization inside living cells. Accumulation and deposition of misfolded amyloid β (Aβ) peptide outside the nerve cells are one of the major causes of Alzheimer's disease (AD). We have developed synthetic breaker peptides derived from the original Aβ sequences that undergo self-cyclization in situ. Such synthetic, breaker peptides showed efficient inhibition and disruption of not only Aβ peptide but related peptides that undergo aggregation.

We are also interested in chemically modified biopolymers derived nanomaterials for drug delivery and live-cell imaging. We have developed various biomaterials fabricated from peptides, nucleic acids and other chemically modified biopolymers as effected tumor-targeting therapeutics including enzyme-prodrug combinatorial therapy and bioimaging.





References:

1. H. Horo, S. Bhattacharya, B. Mandal, L. M. Kundu*, ***Carbohydrate polymers* 2022**, *277*, 118862
2. Ghosh N and Kundu L. M.* ***Future Medicinal Chemistry* 2021**.
3. Ghosh N and Kundu L. M.* ***Bioorganic & Medicinal Chemistry* 2021**, 33, 116017.
4. Horo, H., Saha, M., Das, H.and Kundu, L. M*. ***Carbohydrate polymers* 2021**, 117659.

The Nonlinear Lab: Understanding Complex Natural Phenomenon Through the Study of Chemical Systems

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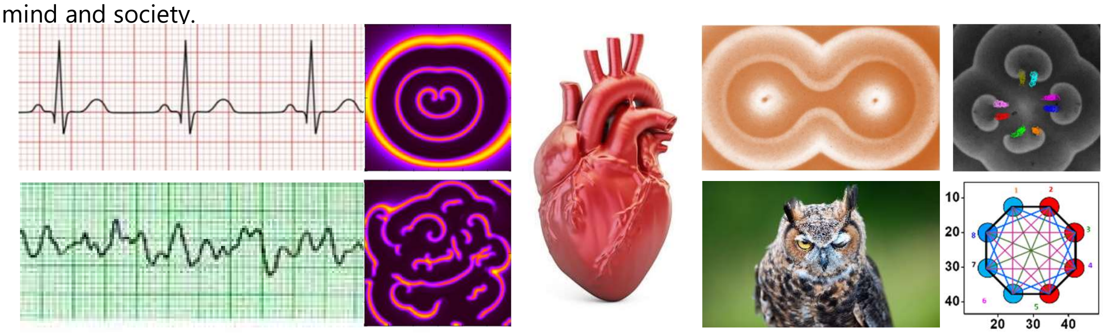
The underlying science behind the static and dynamic patterns seen around us, can be understood by probing into a system that's accessible to us. Some relatively simpler chemical reactions enable us to realize the connection between cell structure and patterns on animal coats, the waves of the heart leading to cardiac arrest and the merger of galaxies. We perform experiments in our laboratory and run simulations on mathematical models, in order to assimilate our results and carry it forward to something more meaningful. Our research is highly multidisciplinary and applies principles of physical chemistry, mathematical biology, physics, engineering, and medicine.

The focus of the NonLinLab at IIT Guwahati is the study of two-dimensional spiral and three-dimensional scroll waves in chemical systems. It is understood that their occurrence in the cardiac tissues leads to the rapid, unsynchronized contraction of the ventricles which thereby reduces the heart's ability to pump blood. This is expressed in the form of medical conditions such as arrhythmia and fibrillation, which may be fatal to cardiac health. Spiral waves also form in the neuronal cortex, and play a major role in uterine contractions. Hence, the understanding and control of these wave forms is of utmost importance. We use the experimental Belousov Zhabotinsky reaction system, to study the spiral and scroll waves. We have been able to unravel some mysteries related to their control and dynamics. We have been successfully able to control these excitation waves by using mild gradients, like thermal, electromagnetic, and concentration gradients. We have also shown that the interaction of these waves amongst themselves can lead to intriguing dynamics, including attraction and annihilation of spirals with opposite chirality. In the presence of heterogeneities, these waves can get anchored leading to an exponential increase in their lifetimes. Pinned spirals can also form chimeras, which may lead to the understanding of complex natural processes, like unihemispheric sleep in some birds and mammals.

In our vision of 2030, we wish to explore more challenging phenomena related to these excitation waves. We expect to see spiral and scroll wave break-up in a real experimental system, that will mimic the Ventricular Fibrillation in the cardiac tissues. We also wish to take forward the control of these waves and initiate new ways to spatially trap them, by using anatomical obstacles or external stimuli. We also expect to be able to find new ways to inhibit chaos in these systems. We believe our future work will lead to newer insights into the behavior of these wave-forms that may pave the way for their control in more complicated biological systems.

We also ponder into more social causes, like dynamic models for understanding human behavior. While we have only taken baby-steps in this direction, we intend to delve into the depths of psychology and social dynamics in the near future, with an aim to contribute our little to the perception of the human mind and society.



Spectroscopy and Dynamics Laboratory

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Our works ranges from understanding basic excited state processes in simple fluorophores to elucidation of photophysical properties of complex nanomaterial, like nanoparticles nanoclusters, carbon dots, perovskite etc. We try to solve long-standing controversies on the origin of luminescence in different materials. . We mainly use fluorescence spectroscopy, FTIR, XRD and TEM. We also apply theoretical tools (quantum mechanical calculations and molecular dynamics simulations) to support experimental results. Some important projects are.

Lead-halide **perovskites** exhibit exceptional optoelectronic properties, which results in their multi-dimensional uses in photovoltaics, light-emitting devices, photocatalysis. However, the soft and polar nature of the perovskite crystals impose severe limitation in their device application due to water and moisture instability. Interestingly, we took advantage of it and demonstrates a controlled chemical transformation of $CsPbBr_3$ to $CsPb_2Br_5$ triggered by nanoconfined water, by placing $CsPbBr_3$ in the non-polar phase within a reverse micelle.[1]

Dual-emissive protein-capped **metal nanoclusters** are emerging nanoprobes for ratiometric sensing. We report a dual-emissive bovine serum albumin (BSA)-capped silver nanoclusters (AgNCs) with a blue emission band at 450 nm and a far-red emission band at 680 nm.[2] We also reported a strategy to synthesize CuNCs with two distinct emission colors from a one-pot reaction mixture. A thiol ligand, mercaptopropionic acid (MPA), was incorporated into a non-luminescent nanoparticle (CuNPs) system prepared from the ascorbic acid reduction of copper salt. Subsequently, the reduction and etching of the non-luminescent system by MPA produces two types of luminescent CuNCs in a time-controlled manner.[3]

Excited-state proton transfer (ESPT) is a sensitive tool for delicate monitoring of structural reorganization, hydration level, and confinement within surfactant and polymer assemblies. For example, we investigate the interaction of a cationic polyelectrolyte, poly(diallyl dimethylammonium chloride) (PDADMAC), with micelles of differently charged surfactants using 8-hydroxypyrene-1,3,6-trisulfonic acid (HPTS) as an ESPT probe.[4] We also utilized ESPT to provide insight into the hydration nature and organization of the non-toxic assembly of a triblock copolymer F127 (poly-(ethylene oxide)101 (PEO101)−poly(propylene oxide)56 (PPO56)−PEO101)) and a zwitterionic sulfobetaine surfactant N-dodecyl-N, N-dimethyl-3-ammoniopropane sulfonate (SB12).[5]

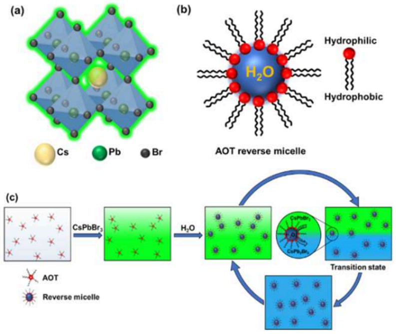


Figure. (a) $CsPbBr_3$. (b) reverse micelle and (c) reversible chemical transformation of $CsPbBr_3$ to $CsPb_2Br_5$ NCs using AOT reverse micellar solution.

References

1. Sahu, S.; Debnath, T.; Sahu, K. Reversible CsPbBr3 ↔ CsPb2Br5 Transformation via Reverse Micellar Aqueous Solution. ***J. Phys. Chem. Lett.* 2024,** *15*, 3677-3682.

2. Sarkar, P.; Nandi, N.; Barnwal, N.; Sahu, K. BSA-Capped Dual-Emissive Silver Nanoclusters for Detection of IO4– and Cu2+ Ions. ***ACS Applied Nano Materials* 2023,** *6*, 15851-15859.

3. Sarkar, P.; Nandi, N.; Barnwal, N.; Sahu, K. Mercaptopropionic acid-assisted synthesis of green and blue emissive copper nanoclusters for multimodal sensing, logic gate, and white light applications. ***Materials Today Chemistry* 2023,** *27*, 101341.

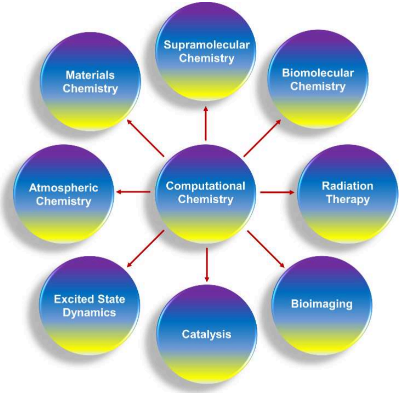
4. Pal, T.; Sahu, K. Exploring cationic polyelectrolyte–micelle interaction via excited-state proton transfer. Signatures of probe transfer. ***Phys. Chem. Chem. Phys*. 2023,** *25*, 2963-2977.

5. Pal, T.; Sahu, K. Effect of salt addition on a triblock copolymer-zwitterionic surfactant assembly: insight from excited-state proton transfer. ***Phys. Chem. Chem. Phys.* 2023,** *25*, 29816-29830.

Computational Approaches to Solve Real-Life Problems

Dr. Manabendra Sarma

The past decade has witnessed several groundbreaking works with Computational Chemistry. In a real system, it is at times difficult to establish the hypothesis with the experimental studies alone, which could be resolved by the use of quantum mechanical approaches and molecular dynamics simulations. Thus, our research group is engaged in various fields of Chemistry. While our main focus lies in pioneering novel theoretical methodologies for laser-assisted control of chemical reactions and the investigation of resonances in electron-molecule scattering, we also explore the fields of supramolecular chemistry, biomolecular chemistry, bioimaging, materials chemistry, atmospheric chemistry, excited state dynamics, and catalysis.



Our group has established the potential of noncovalent interactions (NCIs) in detecting and encapsulating natural hazards and biologically important anions. The role of NCIs is also implicated in the designing of drug molecules for the treatment of Alzheimer’s disease and cancer. The impact of low energy electrons (LEEs) on substituted and unsubstituted DNA subunits and the role of other biologically relevant molecules in DNA damage by LEEs have also been studied. We have spread our research wings to detect the toxic gases in the environment using 2D materials and delve into the mechanism of the environmental impact of chlorofluorocarbons (CFCs). Concurrently, our research focuses on the exploration of transition metal-based complexes and heavy lanthanide elements, with their potential applications in water oxidation and bio-imaging of the human brain, whilst our efforts encompass the development of a model aimed at understanding the turnover number (TON) of transition metal catalysts. Our research findings include non-adiabatic dynamics simulations to observe the bond-breaking/formation, proton transfer, etc., in biologically relevant molecular systems. In the era of energy crisis, global warming, and deadly diseases, our lab intends to contribute to the respective fields through computational approaches. One of our objectives is to convert peptide-based anion receptors into functional materials by combining them with the surface of 2D materials, exploring their properties for sensing applications and designing new 2D materials for electrocatalysis and energy storage. By employing advanced computational models, we aim to unravel the reaction dynamics of the pollutant with air-borne radicals like OH, Cl, and NO_3. Developing new strategies would help to mitigate pollution and safeguard our environment. We will explore photoisomerization processes in small to large photoactive molecular systems and gain insight into the effect on non-radiative phenomena to discern multiple biological applications. We envision contributing to medical science by designing drug molecules for depression, new radiosensitizers for efficient radiotherapy, and developing stable, high-relaxivity lanthanide-based macrocyclic complexes for MRI contrast agents.

References:

1. Sarma, M.; Sarmah, M. P.; Sarma, M. ***Chem. Asian J***. **2024**, e202400880.
2. Bhattacharyya, H. P.; Sarma, M. ***ChemPhysChem*** **2024**, e202400004.
3. Medhi, B.; Nath, U., Sarma, M. ***J. Chem. Phys.*** **2024**, 160, 154308.
4. Medhi, B.; Nath, U., Sarma, M. ***J. Chem. Phys.*** **2024**, 160, 154308.
5. Lama, B.; Sarma, M. ***J. Phys. Chem. B*** **2024**, 128, 6786.
6. Changmai, R. R.; Daimari, S. R.; Yadav, A. K.; Sarma, M. ***Phys. Chem. Chem. Phys.*** **2024**, 26, 23363.
7. Singh, H. K.; Nath, U.; Keot, N.; Sarma, M. ***Phys. Chem. Chem. Phys***. **2024**, 25, 26767.
8. Kumar, S.; Sarma, M. ***Phys. Chem. Chem. Phys.*** **2024**, 26, 25524.
9. Keot, N.; Sarma, M. ***J. Phys. Chem. A*** **2024**, 128, 8346.
10. Daimari, S. R.; Changmai, R. R.; Sarma, M.; ***J. Phys. Chem. A*** **2024**, *128*, 6240.

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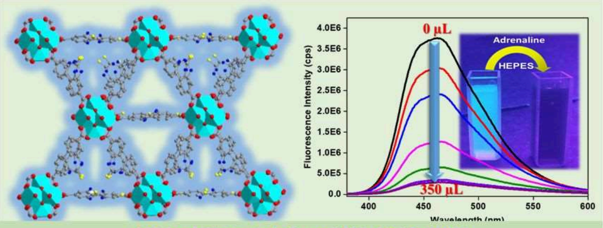
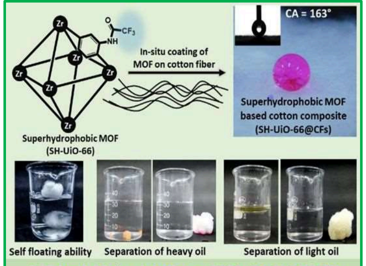
In our research group, we focus on synthesis, characterization and applications of metal-organic frameworks (MOFs) for (i) fluorescence based chemical sensing, (ii) heterogeneous catalysis, (iii) oil/water separation, (iv) anti-bacterial activity, (v) removal of environmental pollutants from wastewater, etc. For fluorescence sensing applications, we synthesized several physicochemically stable, porous and highly luminescent MOFs for the sensing of biologically important analytes (uric acid, adrenalin, hemin, ROS, RNS, ect), metal ions, anions, harmful pesticides, pharmaceutically active drug molecules (anti-cancer, anti-hypertensive, anti-Parkinson, anti-tuberculosis), biological signaling molecules (H_2S, NO, etc.), biomarkers (bilirubin, 3-nitrotyrosine, etc.), biogenic amines, etc. The MOFs with highly π-conjugated organic linkers or fluorophore-anchored MOFs showed highly selective and sensitive fluorometric turn-on or turn-off response for the sensing of various analytes in aqueous phase, gas phase, various pH media, different real samples (water, serum, urine, etc.). In some cases, paper, polymer or fabric based thin film composites incorporating the fluorescent MOF powder were developed for the on-site real-time detection of target analytes. Exceptionally high selectivity, short response time and ultra-low sensitivity have been achieved for the fluorometric detection of most of the target analyes. For few cases, we have been able to carry out the live-cell imaging of the analytes (e.g. H_2S, CN^-, ROS, RNS, uric acid, etc.).



ACS Appl. Mater. Interfaces, 2023, 15, 22, 26843

For oil/water separation, we prepared several fluorinated or fluorine-free (long alkyl chain based) superhydrophobic MOFs. The MOFs composites (with various fabrics or sponges) were utilized for removal of various oils from oil/water mixtures with high separation efficiency and adsorption capacity. Exceptionally high reusability (up to 60th cycles) and remarkable flux for the separation of oil from oil/water mixtures were achieved for some of the superhydrophobic MOF composites. They can be utilized for the adsorption and filtration sequestration of oils from oil/water mixtures. Few of the superhydrophobic MOF composites were employed for separation of hydrophobic drug molecules or pesticides from environmental wastewater with remarkably high adsorption capacity, separation efficiency, great selectivity and high recyclability. Ag nanoparticles have been incorporated on the surface of some of superhydrophobic MOF composites, which displayed remarkable anti-bacterial and bacterial anti-adhesion characteristics. For heterogeneous catalysis, we developed several MOF catalysts for various organic transformations such as Friedel-Crafts alkylation, epoxide ring opening, Friedlander condensation, Biginelli reaction, CO_2 cycloaddition with epoxide, photo-reduction of CO_2, oxidation of thiols, cascade catalysis, etc.



ACS Appl. Mater. Interfaces, 2021, 13, 8563-8573

In the future, we will continue to work on these research areas for environmental protection, safety of foods and human health. The developed MOF sensors (in thin-film or paper strip forms) will be helpful for on-site, real-time monitoring of various environmental pollutants, biological molecules, biomarkers, etc. The MOF based heterogeneous catalysts will be highly useful for the chemical industry for the catalysis of various organic transformation and electrochemical processes (e.g. water splitting). The superhydrophobic MOF composites with foams and fabrics can be used for real oil/water separation (e.g. marine oil spill clean-up).

Supramolecular Dye Chemistry

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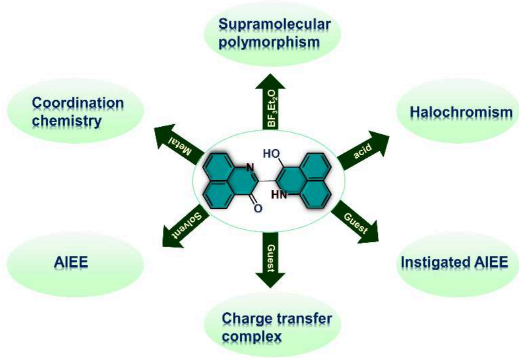
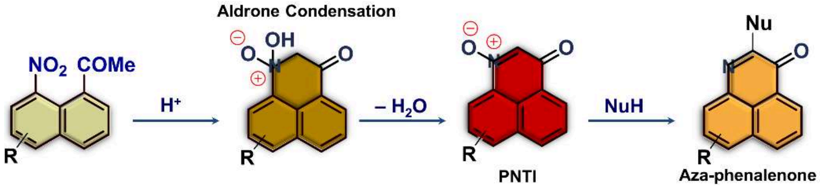
We are die-hard fan of dye molecules and our research group explore the colorful chemistry of N-doped polycyclic aromatic hydrocarbons (PAHs). The electrochemical and optical properties of the PAH dyes are tuned with the help of various non-covalent interactions like metal-coordination, aromatic-interaction, hydrophobic interaction *etc*. We are interested in the supramolecular arrangement of the dyes. We also focus on the medicinal and materials applications of the PAHs. Our current activities are based on the following topics:

- ***peri*-Naphthoindigo (PNI)** is a fascinating dye consisting of four different functional groups sandwiched between two naphthalene rings via *peri*-positions.[1] Although, the structure of its diketo isomer was proposed in 1977 in a patent,[2] the synthesis of PNI remained elusive for several decades. After many unsuccessful attempts, we accomplished its challenging synthesis for the first time in 2018.[1] PNI has quite distinct properties than that of the famous historic dye indigo. PNI shows many interesting properties, including halochromism in acidic media, self-sorting, and aggregation induced enhanced emission (AIEE) phenomenon.[3] However, the most intriguing feature of the dye is its ability to instigate AIEE in other dye that could not show AIEE alone. The boron-difluoride coordinated derivative of the dye (PNI-BF_2) also shows interesting phenomenon like polymorphism in dye aggregates.[4] We aim to contribute further to the intriguing chemistry of PNI.



- **Aldrone condensation** is a newly invented reaction of aromatic nitro group, and defined as the reaction of a C-nucleophile with nitro group to produce aldonitrone via addition-elimination mechanism.[5] With the help our invented reaction, we are able to realize two important class of compounds: *peri*-napthoisatogens (PNTIs) and aza-phenalenone.[5] The first class of compounds show supramolecular switch, while the other dyes show good anti-cancer activities· We aim to increase the substrates scope as well as application aspects of the aldrone condensation.



- **Supramolecular rearragnement in the excited state** is a new phenomenon which gives variable emission properties of a dye as a function of concentration. We wish to contribute further to our new findings.

References:

1. R. J. Das, K. Mahata, ***Org. Lett.*** **2018**, *20*, 5027.
2. R. A; Nathan, R. E. Schwerzel, A. H. Adelman, R. E. Wyant, U.S. Patent 4004572, **1977**.
3. R. J. Das, K. Mahata, ***Soft. Matter.*** **2019**, *15*, 5282.
4. I. Debnath, T. Roy, J. Matern, S. A. H. Jansen, G. Fernandez, K. Mahata.; ***Org. Chem. Front.*** **2021**, *8*, 5432.
5. I. Debnath, T. Roy, K. Mahata, ***Org. Chem. Front.*** **2024**, https://doi.org/10.1039/D4QO01613K.
6. I. Debnath, T. Roy, K. Mahata, ***Chem. Asian J***., **2023**, 18, e202300827.

Exploring Nanofluidic Phenomena Towards a Greener and Safer Future

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Shortage of clean water and inadequacy in sustainable energy are two of the most worrisome yet highly interconnected issues of the modern era. The aim of our research group is focused on finding solutions to this entangled problem. Numerous inventive strategies for excavating energy from alternative resources (like waste mechanical energy, waste heat, evaporation, wind, and wave), and producing clean water in sustainable manners (like forward osmosis and solar thermal evaporation) are being intensely explored based on exclusive properties of liquids and solids confined in nanometer length scale.[1-3] We also aim to address these entangled issues of water and energy as a whole, like synchronized energy harvesting during the forward osmosis process,[4] and harvesting solar energy in the form of drinking water and electrical energy.

Our group also aim to fabricate eco-friendly, cost-effective and naturally abandoned responsive materials with high sensitivity and robustness.[5] As society moves towards more and more automation in areas like health, safety, economic production, and space technology, the search for new materials that can morph in a desirable manner has become a distinct priority. Nature produces a plethora of such materials to accomplish various biological tasks and offers persistent inspiration to design and manufacture artificial smart materials. We explore robust and naturally abundant layered materials to create materials with such exclusive properties.

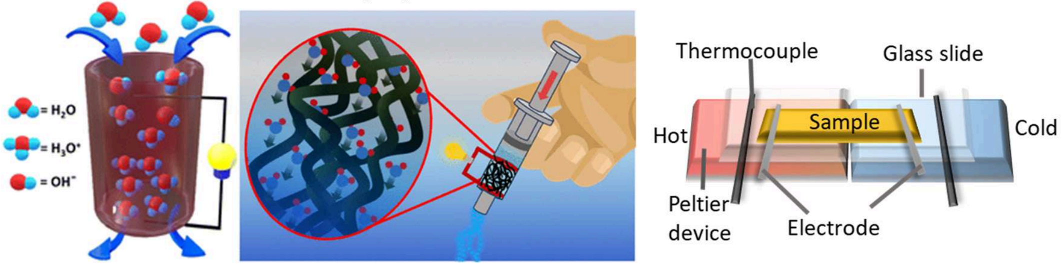

Figure: Schematic representations of strategies of harvesting electrical energy from nanofluidic flow of water.

References:

1. Ionic Thermoelectric Properties of Reconstructed Lamellar Vanadium Pentoxide Membranes, Raktim Gogoi, Harshan Madeshwaran, Arnab Ghosh, Yoav Green, Kalyan Raidongia, ***Advanced Functional Materials***, **2023**, 2301178
2. Application of Lamellar Nickel Hydroxide Membrane as a Tunable Platform for Ionic Thermoelectric Studies, Raktim Gogoi, Arnab Ghosh, Priyamjeet Deka, K. K. R. Datta, and Kalyan Raidongia, ***Materials Horizons***, **2023**, 10, 3072-3081
3. Sustainable electricity from gravity-driven nanofluidic flow of water through modified biochannels of coir fibers, Barsha Rani Bora, Monotosh Mondal, Nabamallika Nath, KKR Datta, Kalyan Raidongia**, *J. Mater. Chem. A***, **2023**, 11, 21383-21392
4. Recovering Electrical Energy from Forward Osmosis Process through Amorphous Silicon Oxide Crosslinked Vanadium Pentoxide-Reduced Graphene Oxide Membrane, Priyamjeet Deka, Sonali Roy, Tukhar Jyoti Konch, Barsha Rani Bora, Raktim Gogoi, Arindom Bikash Neog, Krishnaraajan Sundararajan, Senthilmurugan Subbiah, Kalyan Raidongia, ***Chemical Engineering Journal***, **2023**, 469,143964.
5. Strategic Shuffling of Clay Layers to Imbue Them with Responsiveness, Raj Kumar Gogoi, Kalyan Raidongia, ***Adv. Mater***. **2017**, 29, 1701164.

Catalysis for Sustainable Future

Dr. Dipankar Srimani

The development of new chemical reactions is imperative because they are employed in various chemical processes that provide drugs, fertilizers, fuels, energy and other products, which are essential for human growth and development. The primary factor enabling chemical processes to function so well all around the world is the design of catalysts and the development of novel catalytic techniques. The production of 80% of all manufactured commodities involves catalytic reactions and they also contribute to 35% of the world's gross domestic product. Thus, catalysis is essential not just for promoting economic progress but also for the production of materials that support modern civilization. However, most of these catalytic processes rely on fossil fuels, which negatively impact the environment and human health. The catalytic processes must be continuously evaluated and modified to address this issue and attain better sustainability. In this context, the development of atom-economical, environmentally benign catalytic reactions employing renewable feedstocks would be significant.

A lot of interest has been shown in developing catalytic reactions using de(hydrogenative) techniques because of their potential to combine the benefits of economy and sustainability. We contribute to developing various earth-abundant, non-toxic transition metal complexes with comparatively higher shelf lives that are also efficient for the dehydrogenative construction of C-C and C-heteroatom bonds to synthesize and diversify heterocycles and carbocycles. Tuning the reaction parameters, our developed catalyst also switches the acceptorless dehydrogenation and borrowing hydrogen catalysis to furnish diverse products from the same set of reactants. Finally, by understanding the bond-activation mechanism, we can fine-tune the catalyst design for targeted chemical processes in a green and sustainable manner.

By 2030, we would like to contribute to the following research area for sustainable development

- Developing inexpensive metal complexes for hydrogenation to degrade plastic waste
- Designing new de(hydrogenative) multicomponent reactions to synthesize various carbocycles and heterocycles
- Designing metal-catalyst for utilization of CO_2 in the area of organic transformations
- To synthesize valuable organic scaffolds by merging visible light catalysis with dehydrogenative transformations
- Developing catalyst for converting lignocellulosic-biomass to various value-added products

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1. A. Samanta, P. Behera, A. Chaubey, A. Mondal, D. Pal, K. Mohar, L. Roy, and D. Srimani ***Chem. Commun***., **2024**,60, 4056-4059.
2. B. Sardar, N. Biswas, and D. Srimani ***Organometallics*** **2023**, 42, 55–61.
3. M.Roy, R. Jamatia, A. Samanta, K. Mohar, and D. Srimani ***Org. Lett.*** **2022**, 24, 8180–8185.
4. D. Pal, A. Mondal and D. Srimani ***Catal. Sci. Technol.,*** **2022**,12, 3202-3208.
5. A. Mondal, R. Sharma, D. Pal and D. Srimani ***Chem. Commun*.,** **2021**, 57, 10363-10366.
6. N. Biswas and D. Srimani ***J. Org. Chem.*** **2021**, 86, 15, 10544–10554.
7. K. Das, A. Mondal, D. Pal and D. **Srimani *Org. Lett*. 2019**, 21, 9, 3223–3227.
8. K. Das, A. Mondal and D. Srimani ***Chem. Commun*.,** **2018**, 54, 10582-10585.

Bio-Inspired Polymeric Materials Lab

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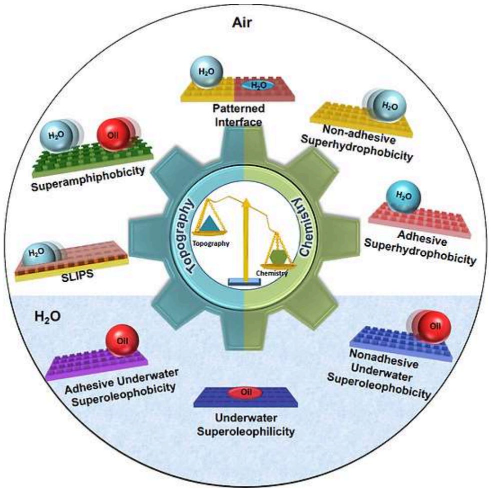
Chemistry and topography are the two distinct tools for customizing different bio-inspired liquid wettability including superhydrophobicity, superamphiphobicity, underwater superoleophobicity, underwater superoleophilicity, and liquid-infused slippery properties. Our lab strategically utilizes facile and robust chemistry to derive materials for functional wettability.

By 2030, we are aiming to address the following relevant challenges;



- We are going to design and explore **wettability pattern interfaces** for antigravity liquid transport, shorting of liquids, moulding of non-aqueous liquids in different shapes, liquid-liquid extraction of molecules at the interface.
- We are going to derive catalyst-free adoptive underwater superaerophobic coating to achieve **energy-efficient hydrogen production**.
- **Ominphobic and reconfigurable capsules** will be attempted to develop for performing droplet chemical reaction—without having adhesion or evaporation loss.
- We are aiming to derive durable and robust underwater superoleophobic coatings for **separating mixtures of liquids independent of their difference in surface tensions.**
- We are aiming to **strategically integrate bio-inspired wettability with a conductive interface** for sensing human motions, tiny vibration, muscle movements at realistic conditions.

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1. Debasmita Sarkar, Manideepa Dhar, Avijit Das, Sohini Mandal, Anirban Phukan and Uttam Manna* "Covalent crosslinking chemistry for controlled modulation of nanometric roughness and surface free energy" ***Chem. Sci.***, **2024**, Accepted Manuscript.
2. Nishanta Barman, Arpita Shome, Saurav Kumar, Priyam Mondal, Karan Jain, Mizuki Tenjimbayashi,* Uttam Manna* "Preprogramming Floating Time of Liquid Marble" ***Adv. Funct. Mater.*, 2023**, 33, 2214840.
3. Angana Borbora,‡ Manideepa Dhar,‡ Arpita Shome, Nishanta Barman, Swaraj Roy and Uttam Manna* "Chemically-Customizing Mechanical Properties and Optical Transparency in Underwater Superoleophobic Coating" ***Adv. Funct. Mater.*, 2023**, 33, 2302569.
4. Angana Borbora, Yang Xu, Souradeep Dey, Xin Wang, Yuxing Yao, Biman B. Mandal*, Xiaoguang Wang * and Uttam Manna* "Lubricated Interfaces Enabling Simultaneous Pulsatile and Continuous Chemical Release Modes" ***Advanced Materials*, 2023**, 35, 2302264
5. Jaysri Das, Subhankar Mandal, Angana Borbora, Sonam Rani, Mizuki Tenjimbayashi* and Uttam Manna* "Modulating Force of Nucleated Hydrogen Bubble Adhesion to Boost Electrochemical Water Splitting" ***Adv. Funct. Mater.*, 2023**, 2311648.
6. Arpita Shome, Avijit Das, Angana Borbora, Manideepa Dhar and Uttam Manna* "Role of Chemistry on Bio-inspired Liquid Wettability" ***Chemical Society Reviews* 2022**, 51, 5452.
7. Manideepa Dhar, Avijit Das, Dibyangana Parbat, Uttam Manna* "Designing a Network of Crystalline Polymer for a Scalable, Nonfluorinated, Healable and Amphiphobic Solid Slippery Interface" ***Angew. Chem. Int. Ed.*, 2022**, 61, e202116763.

Peptide Chemistry Laboratory

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Our research mainly focusses on the development of therapeutic peptides and application oriented smart materials based on peptides and peptidomimetic molecules. We are interested in studying the structure-activity relationships of the biologically active peptides and unravelling their mechanism of action. Some of our research thrust areas are:

Antimicrobial therapeutics:

Microbial infections have been a cause of raising concern in the recent times owing to the rapid development of antimicrobial/ antibiotic resistance in pathogens, that has led to the incapacitation of the arsenal of antibiotics. Antimicrobial peptides are a promising class of compounds with a great potential against the infections caused by the resistant pathogens. Weare interested in developing small highly potent, salt tolerant, non-cytotoxic and protease resistant AMPs, which would be economically viable and extremely slow/incapable of generating resistance against them in the microbes, thus making them efficient therapeutics intackling the microbial infections. We are interested both in *de novo* and MD simulations aidedrational design of the AMPs. We are engaged in studying the mechanism of action of the AMPsin the pathogens in details (experimentally and computationally). We are also interested in probing the structure-activity relationships of the antimicrobial peptides that would enable design of more efficient therapeutics in the future. We are also interested in developing antimicrobial hydrogels that can be applied topically in tackling skin infections and the secondary infections generated around wounds.

Combination Therapy:

In this technique, different therapeutics are employed simultaneously for treating a disease, withan enhanced efficacy, than could be generated by any of the individual therapeutics. We are interested in developing efficient combinations of different AMPs/ Antibiotics and AMPs/ nanoparticles and AMPs that will be effective against resistant microbes. Some of the pathogens can form biofilms, which are usually more challenging to inhibit, more so to eradicate than their planktonic counterparts. We are interested in applying the synergistic combinations developed to tackle the problem of biofilms.

Peptide based smart materials:

Efficacy of the drugs depends on a great extent on their mode of delivery. In our lab, we are interested in developing peptide-based hydrogels/ nanocomposites that can be employed in drug delivery.

References:

1. T. Sarkar, S. Ghosh, P. K. Sundaravadivelu, G. Pandit, S. Debnath, R. P. Thummer, P. Satpati*, S.Chatterjee* Mechanism of Protease Resistanceof D-Amino Acid Residue Containing Cationic Antimicrobial Heptapeptides ***ACS Infect. Dis.*** https://doi.or g/10.1021/acsinfecdis.3c00491.
2. S. Ghosh, T. Sarkar, S. Chatterjee*, P. Satpati* Bridging Thermodynamics, Antimicrobial Activity, and pH Sensitivity of Cationic Membranolytic Heptapeptides–A Computational and Experimental Study ***J. Chem. Inf.Model.,*** **2023**, 63, 2393-2408.
3. G. Pandit, T. Sarkar, S. R.Vignesh, S. Debnath, P. Satpati*, S. Chatterjee* Delineating the Mechanism of Action of a Protease Resistantand Salt Tolerant Synthetic AntimicrobialPeptide against Pseudomonasaeruginosa ***ACS Omega*, 2022**, 18, 15951-15968.

Bioorganic Chemistry Research Laboratory

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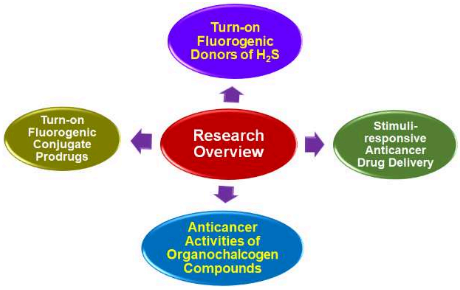
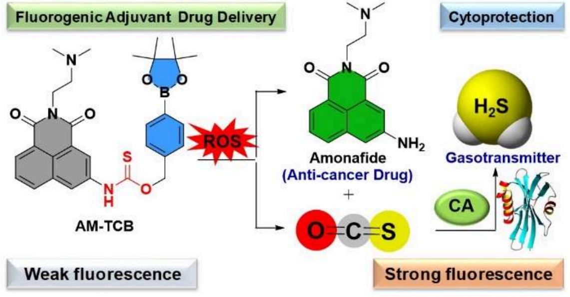


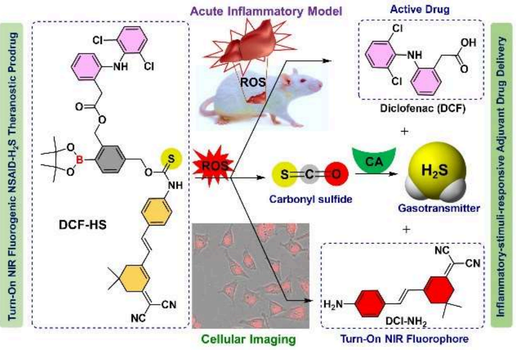
Research interests in our group include the design and synthesis of organic compounds or fluorescently labelled compounds or the turn-on fluorogenic drug delivery systems/prodrugs for the treatment strategies of various diseases such as cancer or inflammatory disorders. We undertake a number of analytical, spectroscopic, kinetic, biochemical and biological (*in vitro* and cellular) methods/strategies to investigate and evaluate the potencies of the rationally designed compounds. Suitable computational approaches are adopted to further support our experimental findings as applicable.

Anticancer Drug Delivery



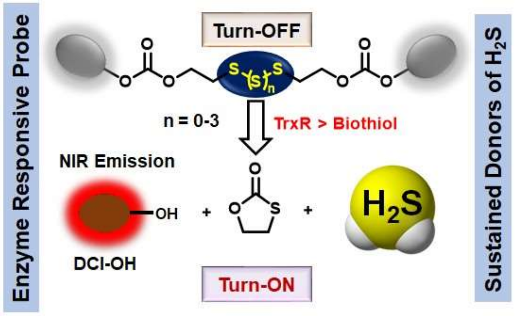
Chem. Commun. **2024**, *60*, 3397-3400.
Chem. Eur. J. **2023**, *29*, e202302197
Chem. Commun., **2023**, *59*, 4802-4805.

Anti-inflammatory Drug Delivery



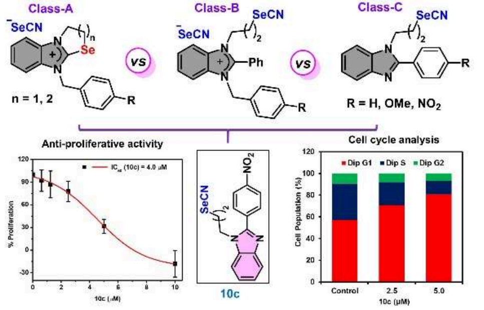
J. Mater. Chem. B **2024** (Advance Article)
Chem. Commun. **2022**, *58*, 7833-7836.

Fluorogenic Donors of H_2S



***J. Mater. Chem. B*, 2022**, *10*, 2183-2193
***Chem. Commun.* 2020**, *56*, 7769-7772
***Chem. Commun.* 2019**, *55*, 13534-13537

Organochalcogen Compounds



***Free Radic. Biol. Med*. 2022**, *191*, 82-96
***New J. Chem*. 2022**, *46*, 11910-11926
***Org. Biomol. Chem*. 2018**, *16*, 8769-8782

By 2030, we aim to rationally develop multi-stimuli-responsive fluorogenic conjugate prodrugs for the delivery of anticancer/anti-inflammatory drugs with gasotransmitters and with minimized drug-induced side effects. The turn-on NIR fluorogenic reporters during the drug delivery will be coupled, which would help monitoring the drug delivery processes with biocompatibility in the in vivo systems.

Organometallics & Catalysis Laboratory

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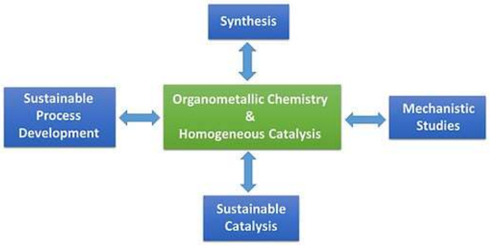
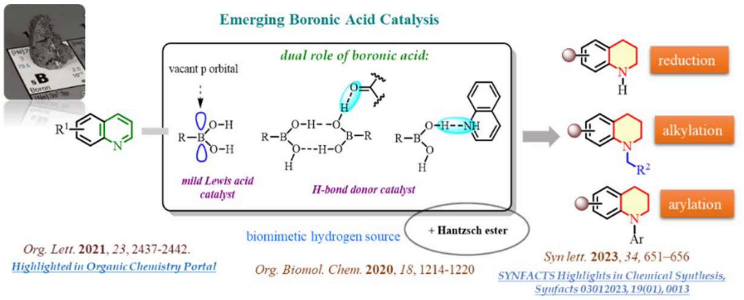
Research interest: Our research involves designing ligands featuring desired features/functionalities, synthesis and reactivity of new organometallic compounds, and the rational development of organometallic catalysts for the activation, functionalization and conversion of challenging substrates to useful chemicals.





Org. Lett. **2021**, *23*, 2437-2442.
Highlighted in Organic Chemistry Portal

Org. Biomol. Chem. **2020**, *18*, 1214-1220

Syn lett. **2023**, *34*, 651–656
SYNFACTS Highlights in Chemical Synthesis, Synfacts 03012023, 19(01), 0013

Selected reference: i) Bhattacharyya, D.; Sarmah, B. K.; Nandi, S.; Srivastava, H. K.; Das, A. ***Org. Lett.*** **2021**, *23*, 869. ii) Adhikari, P.; Bhattacharyya, D.; Nandi, S.; Kancharla, P. K.; Das, A. ***Org. Lett.*** **2021**, *23*, 8390; iii) Sarmah, B. K.; Konwar, M.; Das, A. ***Org. Lett.*** **2021**, *23*, 8390. iv) Adhikari, P.; Hazarika, N.; Bhattacharyya, K; Das, A. ***Org. Lett*****.** **2024**, *26,* 286. v) Konwar, M.; Das, T.; Das, A. ***Org. Lett.*** **2024**, *26*, 1184. vi) Konwar, M.; Hazarika, N.; Das, A. ***Org. Lett.*** **2024**, *ASAP*. 10.1021/acs.orglett.4c00542. vii) D. Bhattacharyya, P. Adhikari, K. Deori, A. Das, ***Catal. Sci. Technol.,*** **2022**, *12*, 5695-5702.

By 2030 we would like to contribute in solving the following issue: Metal-pincer-complexes are expedient tools for organic synthesis. Their long-term stability and easy functionalization have allowed the development of novel catalytic systems that have had a tremendous impact in different areas of chemistry. The current paradigm for the development of metal-pincer catalysts primarily focus on a single active metal site with the ligands that impart steric and electronic tunability to achieve the substrate binding and activation. Nevertheless, less attention has been made to the molecular level understanding of secondary sphere activation of small molecules. Secondary interactions are ubiquitous in biological systems and are largely present in metalloenzymes. Notably, this secondary coordination sphere incorporation allows to stabilize the small-molecule substrate as well as reactive intermediate *via* non-covalent interaction such as hydrogen-bonding as example, Further, it alters redox properties, and promotes functional activity in the system. Owing the motivation of biological system, we interest to develop a new H-bond donors containing metal-pincer system for substrate binding and activation of small molecules in particular we are interested on N_2 centered reduction chemistry, which may contribute mechanistic details for nitrogenase function. Furthermore, finding will pave the way to provide fundamental insights into how green-house gases, such as CO_2, N_2O can be activated assisted by secondary coordination sphere of the metal complex.

Pincer-Base-Metal Catalysis for Generation of Specialty Chemicals, Fuel, Green Hydrogen and Electricity

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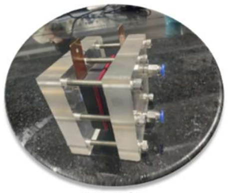
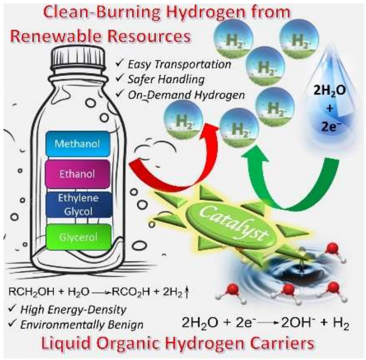
Current global research is greatly focused on the development of greener, sustainable and atom-economical methods for the formation of C-C bonds leading to versatile fuels and value-added chemicals. This greatly negates the typical disadvantages of classical coupling of alkyl halides that generally are accompanied by the formation of hazardous waste. Well explored approaches towards greener and sustainable C–C bond forming reactions involve catalytic C–X (X = H, Cl, Br, I) activation and subsequent cross coupling either involving radical mechanisms or purely organometallic mechanisms. Transition metal catalyzed coupling of alcohols is a promising route to new C-C bonds as they are greener and atom-economical with water as the sole by-product. Typically, these reactions follow the sequence of catalytic dehydrogenation to carbonyl compounds, aldol condensation and a tandem catalytic hydrogenation of the resulting α,β–unsaturated carbonyl compound. This net alcohol alkylation not only leads to the synthesis of versatile organic molecules that find applications as drug molecules, synthetic lubricants, fuels and specialty chemicals but also generates hydrogen as a by-product.

Organometallic complexes have enjoyed great success in catalysing and/or mediating organic transformations which otherwise are not possible. The ease of ligand synthesis along with the ability to tailor the functionalities and ligating atoms have led to a plethora of complexes with a wide variety of metals. This has facilitated one, to pick complexes with desired steric and/or electronic parameters to suit their requirement. For efficient catalysis, it would be desirable to have a subtle balance between catalyst stability and reactivity. In the past four decades, it has been more often found, that pincer-metal complexes perform exceedingly well in striking this balance. With a particular emphasis on base metals, the research group of Dr. Akshai Kumar investigates the pincer-base-metal chemistry and their role in catalyzing C-H activation/functionalization mediated C-C bond formation of alcohols via radical/organometallic pathways that ultimately lead to the synthesis of green hydrogen, high-value fuels and specialty chemicals starting from waste under thermochemical conditions. Attempts are also being pursued to probe the activity of these pincer-metal catalysts under photochemical and/or electrochemical conditions to fabricate Direct Alcohol fuel-cell (DAFC) stacks capable of meeting futuristic low-power and high-power energy demands. Exciting opportunities lie ahead not only in the development of novel methods for the generation of green hydrogen but also in the fabrication of low-cost, high-performance DAFCs containing non-noble, environmentally benign electrode assemblies built using state-of-art technologies.



DAFCs



Frustrated Ion-Pair Catalysis for Carbohydrate Chemistry and Beyond

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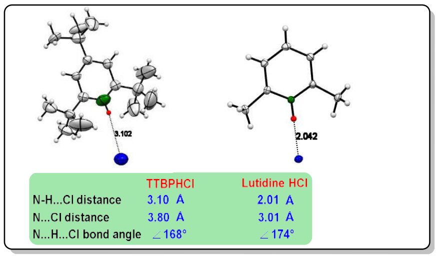
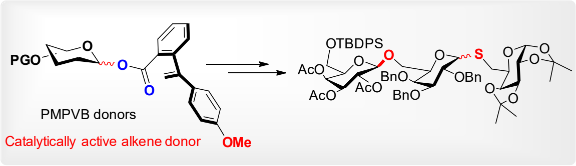
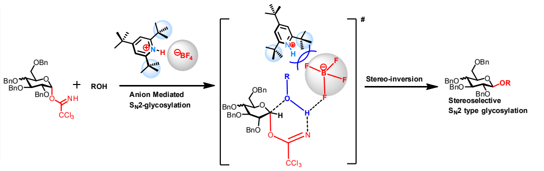


	TTBPHCl	Lutidine HCl
N-H...Cl distance	3.10 Å	2.01 Å
N...Cl distance	3.80 Å	3.01 Å
N...H...Cl bond angle	∠168°	∠174°

Frustrated Lewis pair (FLP) concept over the past decade and a half has emerged as an intriguing strategy, where main group elements can be utilized to activate small molecules. Strained interactions between a sterically bulky Lewis acid and a bulky Lewis base that cannot form a classical LB adduct would activate a third sterically accessible substrate. On similar lines, we hypothesize that Ion-Pairs arising from sterically bulky Bronsted acid and bulky Bronsted base would have strained ion-pair interactions that can be leveraged in ***Frustrated Bronsted Pair (FBP) catalysis***. Interestingly, the analysis of the single crystal X-ray structure of the Bronsted pair TTBPyHCl led to the observation that NH...Cl distance of 3.10 Å (Figure 1) is significantly longer (more than 1 Å longer) than in the analogous, albeit less bulky lutidineHCl in which the NH...Cl distance is 2.01 Å and is beyond any H-bonding interaction. It is clear that chloride is in a strong H-bonding interaction with cation in the later case whereas no such interaction is present in the former. Seminal studies by Andreeva et al. on analogous DTBP also reveal that no such H-bonding exists between the protonated $[\text{DTBP-H}]^+$ and the anion even in the solution state. We hypothesized that the increased separation by almost > 1 Å from the distance of minimum energy between the ion-pair (or Bronsted pair), could result in a certain amount of strain or frustration and may imbue an increased reactivity in both the ions (Frustrated Bronsted pair activity) akin to the frustrated Lewis pairs (FLP). Besides, the N-H...Cl bond angle that should be linear is also deviated to a great extent in the case of the bulky TTBPyHCl to 168˚. Our research is focused on exploiting the "sterically strained" Bronsted pair salts arising from sterically hindered tri-*tert*-butylpyridine with various acids and studying the unique reactivity of these salts in catalyzing various organic reactions. Our group has been investigating this concept of bulky pyridine salts as ***organocatalysts*** particularly in the development of ***stereoselective glycosylation*** reactions. In addition, our group research activities revolve around the developed various new techniques for the *stereoselective glycosylation* reactions and development of *new organic methodologies* with a special emphasis on ***carbohydrate chemistry***.





References:

1. Exploiting the Strained Ion-Pair Interactions of Sterically Hindered Pyridinium Salts Toward SN2 Glycosylation of Glycosyl Trichloroacetimidates. Addanki, R. B.; Moktan, S.; Halder, S. H.; Sharma, M.; Sarmah, B. K.; Bhattacharya, K.; Kancharla, P. K. ***J. Org. Chem.*** **2024**, 89, 3713-3725.
2. TfO–···H–O–H Interaction-Assisted Generation of a Silicon Cation from Allylsilanes: Access to Phenylallyl Ferrier Glycosides from Glycals. Addanki, R. B.; Halder, S. H.; Kancharla, P. K. ***Org. Lett.*** **2022**, 24, 1465-1470.
3. Glycosyl Ortho-[1-(p-MeOPhenyl)Vinyl]Benzoates (PMPVB) as Easily Accessible, Stable, and Reactive Glycosyl Donors for O-, S- and C-glycosylations Under Brønsted Acid Catalysis. Halder, S. H.; Addanki, R. B.; Moktan, S.; Kancharla, P. K. ***J. Org. Chem.*** **2022**, 87, 7033-7055.
4. C–H···Anion Interactions Assisted Addition of Water to Glycals by Sterically Hindered 2,4,6-Tri-tert-butylpyridinium Hydrochloride. Mukherji, A.; Kancharla, P. K. ***Org. Lett.*** **2020**, 22, 2191-2195.

Computational Material Chemistry (CMC) Lab

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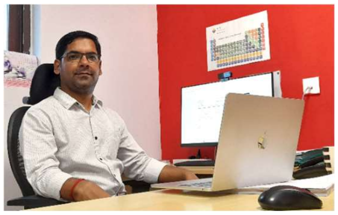

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To address climate change and meet the targets set by the Paris Agreement, such as reducing greenhouse gas emissions by 45% by 2030 and achieving net zero emissions by 2050, it is imperative to reduce our heavy reliance on fossil fuels in modern societies. Electrocatalysis offers a potential solution to this challenge, providing a way to produce fuels and chemicals sustainably. While the research community is increasingly interested in using electrocatalysis, current electrocatalysts are not yet efficient enough to make these processes economically viable. Thus, there is a significant challenge in developing new electrocatalysts for energy transformation. A deep understanding of the atomic-scale processes that control reactivity is essential for progress toward a sustainable energy future.

The **Computational Material Chemistry Laboratory** focuses on using ab initio computational methods to simulate reactions that occur at the electrode-electrolyte interface, which is a critical component in an electrochemical cell. Understanding the atomic-scale details at this interface could greatly impact the rational design of fuel cells, batteries, and other energy conversion systems, such as the electroreduction of carbon dioxide. Our current research projects include:

Computational Modeling of the Local Reaction Environment in Electrocatalytic Media: Gaining insights into the specific reaction environment at interfaces between catalysts and electrolytes is essential for evaluating dynamic processes in electrochemical energy research. Sophisticated theoretical and computational methods, such as machine learning, will play a key role in unraveling this environment under real-world conditions. This understanding will be critical for the design and selection of catalyst materials, as well as the optimization of electrode configurations, to achieve optimal performance and stability.

Theoretical Modeling of Single-Atom Electrocatalysis: Single-atom catalysis (SAC) provides a high level of control and tunability due to its precise, uniform single-atomic sites. This allows for the establishment of clear structure-performance relationships and the development of designing and enhancing catalysts. However, there are challenges in formulating these understandings, as recent research indicates that factors such as the symmetry of frontier orbitals and electrostatic interactions can have a substantial impact on catalysis, occasionally conflicting with conventional theories.

Machine Learning for Heterogeneous Catalysis: Efficient electrocatalysts play a crucial role in producing hydrogen through water electrolysis. However, the traditional trial-and-error method for developing advanced electrocatalysts is not only costly and time-consuming but also labor-intensive. Thankfully, the emergence of machine learning provides new avenues for discovering and designing electrocatalysts. By analyzing both experimental and theoretical data, machine learning can effectively predict the performance of electrocatalysts in the hydrogen evolution reaction (HER). The potential of machine learning in heterogeneous catalysis research is just beginning to be tapped, with significant room for further advancement. Our research group is using machine learning to: (1) expedite the screening of catalysts; (2) identify structure-property relationships in catalytic data; (3) develop interatomic potentials for rapid catalyst simulation; and (4) investigate catalytic mechanisms.

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References:

1. K. Bhattacharyya et al. ***J. Phys. Chem. C*, 2022**, 126, 18623-18635.
2. K. Bhattacharyya et a. ***J. Phys. Chem. C* 2021**, 125, 4379-4390

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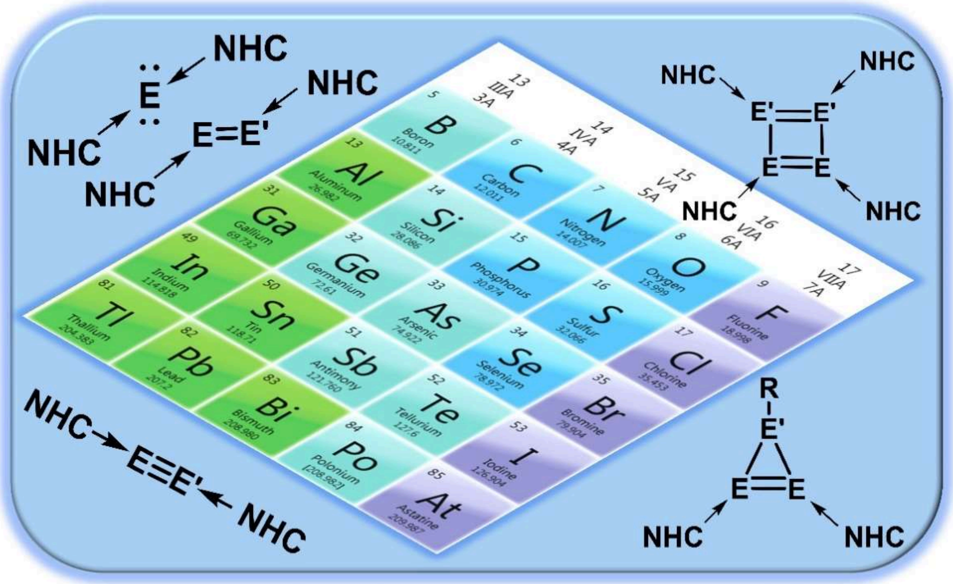
The advent of the 21st century has witnessed enormous attention in developing compounds with low-valent main-group elements due to their interesting electronic features and unusual reactivities. The theoretical study has revealed that compounds with the low valent main group centered such as heavier carbene homologous, homo/heteroatomic multiple bonded compounds, and radicals possessing smaller HOMO-LUMO gaps are enabled to activate small molecules (e.g. H_2, NH_3, CO_2, etc.), which was previously considered the domain of transition metal complexes. Thus, utilizing these molecules as a catalytic alternative to the expensive transition metals is one of the sole goals of the organometallic chemist. However, isolation of these compounds under the ambient temperature is a challenging task due to their inherent reactivities and tendency to undergo oligomerization or polymerization.



Therefore, coherent steric and electronic stabilization factors are required to stabilize these molecules. In our research group, we will explore the chemical tricks for taming the transient group 13 and group 14 low-valent and radical compounds.[1] Additionally, our group will work on the rational designing, synthesis, structure, bonding, and unusual reactions of the carbon-free π-aromatic molecular systems. Moreover, we will explore the synthesis, photo-physical properties, and applications of boron-doped conjugated molecules. The continued development of boron-doped conjugated materials holds great promise for the realization of efficient and versatile optoelectronic device applications.[2]

References:

(1) ***J. Am. Chem. Soc.*** **2023**, *145*, 21475–21482; ***Angew. Chem.*** **2021**, *59,* 23015–23019; (2) ***Nat. Chem.*** **2024**, *16*, 437–445; ***J. Org. Chem.*** **2022**, *87*, 3967–3977.

Computational Material Science and Biomaterials Lab

Dr. Debdas Dhabal

Research area: Computational Material Science, Microporous Materials, Smart Polymers, Enhanced Sampling, Machine Learning, Theory of Liquids
Website: https://sites.google.com/site/debdasdhabal/home

The development of novel, efficient computational methods that complement experimental data is crucial across various disciplines, such as biomedicine, material design, food engineering, and atmospheric sciences. Over the past few decades, molecular simulations have emerged as a valuable tool for unraveling microscopic mechanisms underlying multiscale phenomena, enabling the design of task-specific materials. Nonetheless, there is still significant room for improvement in constructing techniques capable of accurately and efficiently elucidating the fundamental principles governing these molecular processes. Our group uses molecular simulations, enhanced sampling, machine learning, and theory to develop computational approaches for designing advanced functional materials.

Vision 2030

Stimuli-responsive polymer materials for controlled drug-delivery and release systems:

Stimuli-responsive polymer materials play an increasingly important part in a diverse range of biomedical applications, such as controlled and targeted drug delivery, tissue engineering, and peptide separation, as well as biosensors. An important characteristic of stimuli-responsive polymers is their reversible phase separation in response to the external stimulus-triggered change in solubility. Our goal is to investigate a molecular-level mechanism of its phase separation that in turn would help to develop better stimuli-responsive polymeric drug-delivery systems with sustained and controlled drug-release properties.

Metal-organic framework (MOF) materials with tailored properties:

Because of their tunable porosity, microporous materials such as metal-organic frameworks (MOFs) have widespread uses in adsorption, catalysis, separation, purification, and energy storage. Synthesis of new MOF materials mostly relies on the "trial and error" approach of selecting new chemical species and the reaction conditions. Therefore, a major leap forward toward a predictive synthesis requires a general formalism underlying MOF crystallization, rather than a case-by-case empirical optimization. We plan to develop accurate and efficient multi-scale molecular dynamics models for the study of the nucleation and growth of MOFs.

Green materials with superior deicing and anti-icing propensity: Controlling the heterogeneous nucleation of ice is a central challenge to industries related to snowmaking, artificial cloud formation, and aircraft. Accumulation of ice on aircraft's wings, climate prediction devices, and wind turbines can often cause serious trouble which results in their low efficiency. Out of many deicing techniques used, chemical deicing is the popular one, but it exhibits environmental drawbacks. For example, widely used propylene glycol is generally regarded as safe but it increases biological oxygen demand (BOD) which harms the environment. Hence, environmentally benign deicers are sought. We plan to use machine learning in conjunction with molecular dynamics simulations to design molecules with efficient anti-icing and deicing properties.

References:

Dhabal *et al*. ***J. Phys. Chem. B.,*** 2022, 127, 2847, Dhabal *et al*. ***Angew. Chem. Int. Ed.,*** **2022**, 61, e202205095, S. Banik, Dhabal *et al* ***npj Comp. Mat.,*** **2022**, 9, A. A. Bertolazzo and Dhabal *et al*. ***Phys. Chem. Lett.,*** **2021**,13, 977, Dhabal *et al*. ***J. Phys. Chem. C.,*** **2021**, 125, 26857, Dhabal *et al*., ***J. Phys. Chem. B.,*** **2021**, 125, 5434.


CAMPUS MAP
INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
To Guwahati
NH-31
To Rangiya
Agiathuri Railway Station
N.F.Railways Track
Agiathuri RoB MAIN GATE
MAIN ENTRY
B Type
A Type
C Type
Community Hall
D Type
F Type
E Type
Lake Serpentine
Children's Park
Hospital
Guest House Extension
Guest House
A.S.E.B GATE
Akshara School
SAC Extension
Married Scholars
Girls' Hostel 2
Market Complex
View Point
Director's Bungalow
Coconut Groove
Subansiri
Indoor & Gym
Football Field
Athletic Field
Power House
Tennis Court
Hockey Field
Volley ball
Basket ball
Food Court
Swimming Pool
Ghorjan River
Boys' Hostel 11
Technology Complex
Incubation Centre
Biotech Park
Conference Hall
Auditorium
Administrative Building
Library
Computer Centre
Lecture Halls
Cricket Field
Boys' Hostel 10
Community Hall
Siang
Manas
Kapili
Dihing
Dibang
Kameng
Barak
Umiam
Sewage Treatment Plant
Brahmaputra
AC Plant
Staff Canteen
Mechanical Workshop
ME
DD
MA
CET
CSE
HSS
EEE
ACADEMIC COMPLEX
CIF
C4
CH
C2 & C3
BT
CL
PH
CE
Demo Earthquake Resistant Building
CE Extension
Water Treatment Plant
KV Quarters
KV Play ground
KV Auditorium
KV School
FACULTY GATE
To Doul Govinda Temple & Ferry Ghat
Lothia Baghicha GATE
PWD ROAD
Mandir
From Rangiya
To Guwahati
From Saraighat Bridge
N
Brahmaputra River
Guwahati City
INDEX
ACADEMIC COMPLEX
DEPARTMENTS
ME Dept of Mechanical Engg
DD Dept of Design
MA Dept of Mathematics and Computing
CSE Dept of Computer Science and Engg
HSS Dept of Humanities And Social Sciences
EEE Dept of Electrical Engg
CL Dept of Chemical Engg
CH Dept of Chemistry
BT Dept of Bio - Technology
PH Dept of Physics
CE Dept of Civil Engineering
CENTRES
C1 Centre for Educational Technology
C2 Centre for Nano Technology
C3 Centre for Energy
C4 Centre for Environment
CIF Central Instruments Facilities
CMMC Centre for Mass Media Communications
SCHOOLS
Kendriya Vidyalaya
Akshara School
MAIN BUILDINGS
HOSPITAL
RESIDENCES
HOSTELS
STUDENT ACTIVITY CENTER (SAC)
OTHER BUILDINGS
BUILDINGS UNDER CONSTRUCTION
ENTRY GATES
BUS STOP
RAILWAY COUNTER & POST OFFICE
CANARA & SBI - BANK/ATM
BRIDGE
WATER BODIES
HILLS