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SCS Annual symposium

2025

Indian Association for the Cultivation of Science

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ROYAL SOCIETY OF CHEMISTRY

ACS Chemistry for Life®

Day 1, 21 February Venue: CV Raman Hall, IACS	
9:15-9:30 am	**Address by the Chair, SCS**
Chair: Tapan K Paine	
9:30-10:20	**Plenary Lecture:** Pradyut Ghosh, IACS
10:20-10:50	**Invited lecture:** Biswarup Chakraborty, IIT Delhi
10:50 – 11:20	**Keynote lecture:** Samik Nanda, IIT Kharagpur
Tea break	
Chair: Prasanta K Das	
11:30-12:00	**Keynote lecture:** Priyadarshi Dey, IISER Kolkata
12:00-12:20	**Invited lecture:** Nabanita Deb, IACS
12:20-12:40	**Invited lecture:** Samit Guha, Jadavpur University
12:40-1:00	**Invited lecture:** Sourav Chakraborty, IIT Tirupati
1:00-2:30	**Lunch**
Chair: Rajib K Goswami	
2:30-3:00	**Keynote lecture:** Nitin Patil, IISER Bhopal
3:00-3:30	**Keynote lecture:** Dattatraya Dethe, IIT Kanpur
3:30-3:50	**Invited lecture:** Durga Prasad Hari, IISc Bangalore
4:10-4:30	**Invited lecture:** Amit Kumar, IIT Patna
4:30-4:50	**Invited lecture:** Debasish Adhikari, IISER Mohali
Tea Break	
5:00-6:30	**Student Flash Presentations*** **(ACS best student-presentation award)**
7:00 -10:00	**Banquet Dinner**

Day 2, 22 February Venue: CV Raman Hall, IACS	
Chair: Arindam Banerjee	
9:30-10:20	**Plenary Lecture:** James McKusker, Michigan State University **Chemical Science (RSC) lecture**
10:20-11:10	**Plenary Lecture:** Hiroyuki Furuta, Kyushu University
Tea break	
Chair: Sudip Malik	
11:20-11:50	**Keynote lecture:** Siddhartha Sarma, IISc
11:50-12:20	**Keynote lecture:** Chandrabhas Narayana, JNCASR
12:20-12:40	**Invited lecture:** Veerabhadrarao Kaliginedi, IPC, IISc
12:40-1:10	**Keynote lecture:** Sourav Dutta, TIFR Mumbai
1:10-1:30	**Invited lecture:** Vivek Tiwari, SSCU, IISc
1:30-2:40	**Lunch**
2:40-4:00	**Poster session**
Chair: Biman Jana	
4:00-4:50	**Plenary Lecture:** Debashree Ghosh, IACS
4:50-5:10	**Keynote lecture:** Jagannath Mondal, TIFR, Hyderabad
5:10-5:40	**Keynote lecture:** Arnab Dutta, IIT Mumbai
5:40-6:00	**Invited lecture:** Susmita Roy, IISER Kolkata
6:00-6:20	**Invited lecture:** Soumya Ghosh, TIFR Hyderabad

Anion Recognition through σ-hole interactions

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ABSTRACT

Selective recognition, sensing and efficient extraction of inorganic anions from aqueous medium is of great importance for promising analytical, industrial and environmental applications. In this direction, in recent years, significant advances have been made in the design of superior supramolecular anion receptors having Sigma-hole (σ-hole) interactions, in particular halogen bonding (XB) and chalcogen bonding (ChB) where a positively charged region on a polarised, electron deficient halogen or chalcogen atom (the σ-hole) interacts with the Lewis base (anion). In this talk, I will discuss on our recent development in the area of anion recognition chemistry, which particularly deals with the XB/ ChB based receptors for (i) selective removal of bromide and iodide,[1-3] (ii) selective sensing of phosphates[4-6] and (iii) selective extraction of perrhenate.[7-8]

KEYWORDS:

Chemical Sensing, Extraction, Inorganic Anions, Halogen Bond, Chalcogen Bond

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Structure prediction from melanin spectra and its photophysics

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Abstract: Melanin is a biopolymer pigment playing a central role in skin photoprotection. Its extensive chemical and dynamic heterogeneity impart this property through a broad featureless ultraviolet/visible absorption spectrum. In this talk, I am going to discuss the inverse learning approach to predict the contributions of dominant chromophore units and structural motifs to different regions of the broad spectrum of melanin. Furthermore, we also discuss the details of photophysics of melanin and the role of heterogeneity in it.

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1. Computational aspects towards understanding the photoprocesses in eumelanin, D. Ghosh, WIREs Computational Molecular Science, 11(3), e1505 (2021).

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The Photophysics and Photochemistry of First-row Transition Metal Complexes: Quantum Coherence, the Marcus Inverted Region, and Applications in Excited-state Chemistry

James K. McCusker
Department of Chemistry, Michigan State University

There has been considerable renewed interest in the photophysical properties of first-row transition metal complexes, driven in part by a long-standing desire to shift to earth-abundant materials for a variety of photolytic applications. A significant challenge to achieving this goal is the fundamental difference in the excited-state properties of first-row metal complexes as compared to their second- and third-row congeners subsequent to light absorption.[1] Our group has been working on understanding the origins of this difference in an effort to develop design principles that will assist in overcoming these intrinsic challenges and develop new paradigms for the creation of photo-active first-row chromophores for applications in solar energy conversion strategies as well as photoredox catalysis.

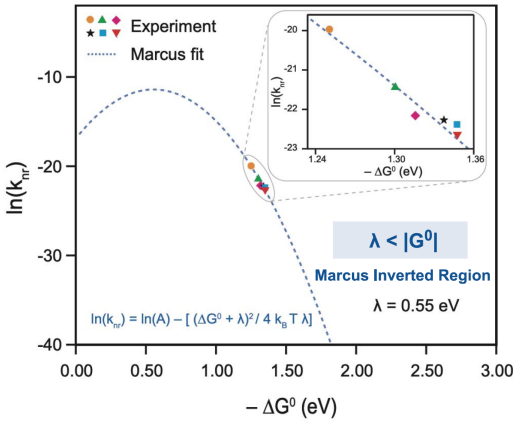

Figure 1. *Photophysical data on a series of Co(III) polypyridyl complexes. The data reveal that the excited-state relaxation dynamics of this class of compounds occur in the Marcus inverted region, which allowed for their application in photoredox-catalyzed C-N bond formation chemistry. From ref. 5.*

This presentation will provide a brief survey of the work we have been engaged in over the past several years employing a combination of synthetic chemistry and ultrafast spectroscopy. Our primary focus has been on compounds involving metals with a d^6 valence electronic configuration.[2] In the case of Fe(II), leveraging information from vibronic coherence was found to provide what amounts to a roadmap for effective synthetic design to lengthen the lifetime of MLCT excited states,[3] whereas the excited-state redox activity of Co(III)-based ligand-field excited states[4] coupled with dynamics occurring in the Marcus inverted region[5] (Figure 1) enabled previously unforeseen applications in photoredox catalysis.[6] Future directions of our research efforts in each of these areas will also be discussed.

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N-Confused porphyrinoids:

Directional evolution from porphyrin isomer to functional NIR dyes

Hiroyuki Furuta[1,2,3]

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Porphyrin derivatives and their analogs show great potential as near-infrared (NIR) chromophores, paving the way for innovative optical materials across various fields, including light-harvesting, sensing, and therapeutic applications. Structural modifications, such as core expansion, peripheral fusion, and chromophore array, have shifted the light-responsive wavelength into the NIR window while maintaining high photo- and chemical stability. Since the discovery of the porphyrin isomer known as N-confused porphyrin, our research group has focused on developing a series of π-conjugated porphyrin analogs incorporating "N-confused" pyrrole rings. These unique structures enhance metal coordination ability, which is crucial for triggering molecular orbital mixing and tuning in N-confused porphyrinoids. This leads to remarkable NIR optical properties and controlled excited-state dynamics.

This presentation will highlight the recent advancements in bis-metal complexes of N-confused porphyrinoids that exhibit NIR functionality, following a brief overview of the chemistry of N-confused porphyrin and its contracted or expanded analogs.[1, 2] Unique properties—including distinct emission and photoacoustic signals in the second and third NIR regions, stable π radicals, an exceptionally high two-photon absorption cross-section upon second NIR pulse irradiation, and numerous metal-ligand charge-transfer transitions via d-π orbital interactions—are all attributed to the molecular orbital features.

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[2] Białek, M. J.; Hurej, K.; Furuta, H.; Latos-Grażyński, L. *Chem. Soc. Rev.* **2023**, *52*, 2082–2144.

Biography:

Hiroyuki Furuta received his B.Sc. (1980), M.Sc. (1982), and Ph.D. (1986) degrees from Kyoto University. After postdoctoral research at the Mitsubishi-Kasei Institute of Life Sciences, Tokyo, and the University of Texas, Austin, he started his independent academic career in 1992 as an Associate Professor at Oita University. In 1997, he moved to Kyoto University as an Associate Professor. In 2002, he was named a Full Professor in Chemistry at Kyushu University. In 2022, he became Professor Emeritus. He has been a Distinguished Professor at Shanghai University and Distinguished Visiting Professor at IIT Kanpur since 2025. His current research focuses on the synthesis of N-confused porphyrinoids with novel functionality.

Stereoselective Cationic Polymerization of Vinyl Ethers Using BINAM-Based Catalysts

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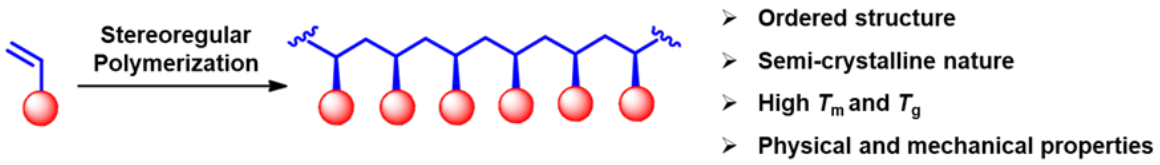
Abstract: The thermomechanical and optical properties of polymers are significantly influenced by their stereochemistry. Therefore, controlling tacticity is crucial in polymer synthesis. Notably, the synthesis of poly(vinyl ethers) (PVEs) can only be achieved through cationic polymerization.[1] However, existing methods for synthesizing isotactic poly(vinyl ethers) (PVEs) are limited to the use of strong Lewis acids, which require high catalyst loadings and restrict the range of monomer substrates available for polymerization.[2] In this study, we demonstrate a novel Lewis acid-catalyzed, stereoselective polymerization of vinyl ethers. Our single-step synthesized ligand provides a stable catalytic system for initiating vinyl ether polymerization, while also serving as a chiral conjugate base to direct the stereochemistry of monomer addition to the ion-reactive chain end. This method allows for an expanded substrate scope compared to previous techniques. Additionally, it enables the use of chain transfer agents to lower catalyst loadings and facilitates catalyst recycling for multiple polymerization cycles. By overcoming the limitations of existing methods, our approach offers a more efficient and versatile pathway for the synthesis of isotactic poly(vinyl ethers) (PVEs) (Scheme 1), enhancing their potential as semi-crystalline thermoplastics with desirable mechanical properties.



Scheme 1. Schematic representation of synthesis of poly(vinyl ether)s by cationic polymerization.

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Harnessing Synthetic Innovation for Complex Natural Products and Therapeutic Discovery

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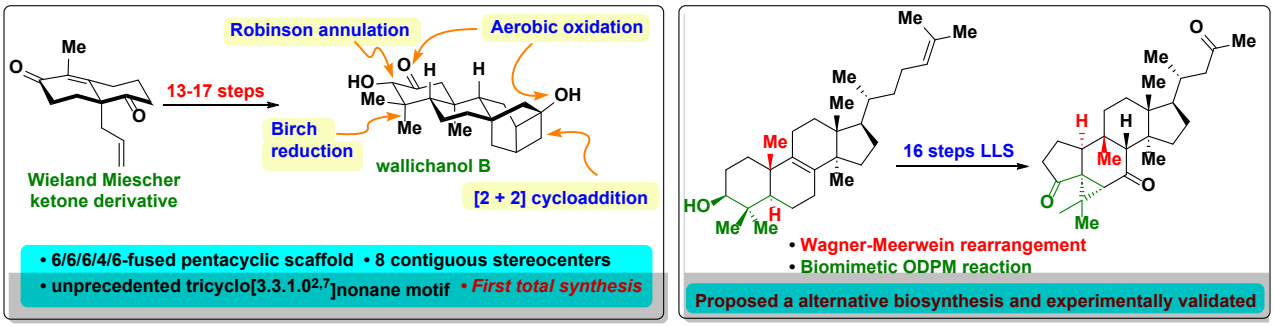
Abstract

This presentation highlights our efforts in the enantioselective synthesis of structurally complex natural products and their therapeutic potential. We achieved the first 13-17 steps enantioselective total syntheses of rearranged *ent*-trachylobane diterpenoids, including (-)-wallichanol A, (-)-wallichanol B, and (-)-sanguinolane, via a novel intramolecular [2+2] cycloaddition, selective alkene reduction using hydrogen atom transfer, and aerobic oxidation strategies. We constructed unique pentacyclic frameworks containing a tricyclo[3.3.1.0^{2,7}]nonane motif.[1,2] Concurrently, we explored the molecular editing of steroids to synthesize cucurbalsaminone A and its analogues, showcasing a biomimetic pathway from lanosterol. This approach incorporated oxidative olefin transposition, oxa-di-π-methane rearrangement, and selective migrations, enabling the discovery of potent antiproliferative agents targeting hepatocellular carcinoma. Mechanistic studies revealed their ability to induce oxidative cell death, offering valuable insights into the synthesis of complex triterpenoids and novel therapeutic candidates.[3] Together, these projects demonstrate the power of innovative synthetic strategies in unraveling natural product complexity and advancing medicinal chemistry.



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Ligand-Enabled Redox Gold Catalysis

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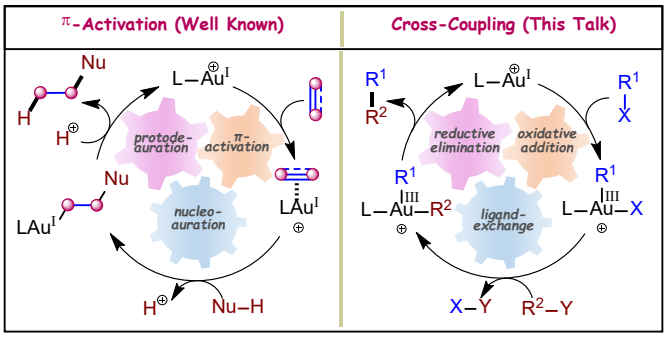
Abstract

Traditionally, gold complexes have been recognized as Lewis acid catalysts for the activation of C-C multiple bonds (Scheme, LHS). Over the years, there has been a considerable shift, and Au(I)/Au(III) redox catalysis is now recognized as an established technique for achieving cross-coupling reactivities (Scheme, RHS). The pioneering work by Zhang and Toste group revealed the role of external oxidants to overcome the high redox potential of Au(I)/Au(III) couple (E0 = +1.41 V) and to facilitate two-electron redox cycle in gold catalysis. Later, the Glorius group introduced the merged gold/photoredox strategy to circumvent the need for a stoichiometric oxidant in these processes. Recently, ethynylbenziodoxolones (EBXs) have also been used for accessing redox gold catalysis serving dual role as oxidant and alkyne surrogate.

All the above strategies were not amenable to the use of aryl halides, and thus their use in gold-catalyzed cross-coupling reactions remained forbidden. In recent years, ligand-enabled gold-catalyzed organic reactions have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will discuss our most recent work on alkene functionalization employing cross-coupling reactivities.



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Slow conformational exchange between partially folded and near native states of Ubiquitin: Evidence for a multi-state folding model

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Abstract

The mechanism by which small proteins fold, i.e., via intermediates or via a two state mechanism is a subject of intense investigation. Intermediate states in the folding pathways of these proteins are sparsely populated due to transient life-times under normal conditions rendering them transparent to a majority of the biophysical methods employed for structural, thermodynamic and kinetic characterization, which attributes are essential for understanding the cooperative folding/unfolding of such proteins. Dynamic NMR spectroscopy has enabled characterization of folding intermediates of ubiquitin that exist in equilibrium under conditions of low pH and denaturants. At low pH, an unlocked state defined as N' is in fast exchange with an invisible state, U'' as observed by CEST NMR. Addition of urea to ubiquitin at pH 2, creates two new states F' and U', which are in slow exchange ($k_{F' \rightarrow U'} = 0.14$ s^{-1} and $k_{U' \rightarrow F'} = 0.28$ s^{-1}) as indicated by longitudinal ZZ-magnetization exchange spectroscopy. High resolution solution NMR structures of F' show it to be in an "unlocked" conformation with measurable changes

in rotational diffusion, translational diffusion and rotational correlational times. U' is characterized by the presence of just the highly conserved N-terminal β1-β2 hairpin. The folding of ubiquitin is cooperative and is nucleated by the formation of N-terminal β-hairpin followed by significant hydrophobic collapse of the protein core resulting in the formation of bulk of the secondary structural elements stabilized by extensive tertiary contacts. U' and F' may thus be described as early and late folding intermediates in the ubiquitin folding pathway.

Green Hydrogen: A Mitigation Strategy

Arnab Dutta

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The energy crisis is a daunting global problem that calls for innovative and sustainable solutions to assure future energy security and environmental stability. To counter this energy uncertainty, accelerating green hydrogen production stands as a vital option to foster carbon-neutral energy infrastructure. This talk will convey an overview of worldwide hydrogen generation techniques, highlighting the key features, indicating the pros and cons, and unravelling the potential environmental consequences. Herein, the conventional grey and cutting-edge green hydrogen production technologies are compared, with a focus on sustainable water electrolysis utilizing renewable energy sources. The existing difficulties with conventional electrolysis, including the usage of expensive catalysts in both cathode and anode, will be discussed, along with the possible gateway with cost-effective and sustainable electrocatalysts.

Substrate recognition and liquid-liquid phase separation of Intrinsically Disordered Protein via Computer simulation

Prof. Jagannath Mondal
Tata Institute of Fundamental Research Hyderabad, India

Intrinsically disordered protein (IDP) presents a frontier to explore due to its enigmatic function. The seminar will present our group's efforts to decipher the recognition process of drug-like molecules by an well-known IDP alpha-synculein. We will present an integrative, machine learning-based approach that, in combination with a Markov State model, identifies key ligand-bound states of this IDP.

In the second part of the seminar, we will explore our efforts to understand liquid-liquid phase separation process of IDP via computer simulation. In particular, we will demonstrate the computer simulation's ability to dissect the role of microenvironments in the form of crowded and saline media as well hydrotropes such as ATP on condensation process of IDP. The presentation will conclude by showing glimpses of generative artificial intelligence in understanding molecular grammer inherent in IDPs.

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Sarkar et al eLife(2024)

Studies of quantum state controlled cold collisions and cold chemistry

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Abstract:

Temperature is a measure of kinetic energy. At very low temperatures, the kinetic energy tends towards zero and, therefore, the potential energy i.e. the interaction energy, however small, plays a dominant role in determining reaction outcomes. Typically, the interaction potential $V(R)$ varies inversely with the interparticle separation R e.g. $V(R) \sim 1/R^6$ for van der Waals interaction, $V(R) \sim 1/R^3$ for dipole-dipole interaction and so on. In dilute gases, the interparticle separation R is large (typically several orders of magnitude larger than the size of the individual atoms) and therefore the interaction is typically weak. The effect of these "weak" interactions can be precisely studied when the gas is cooled to sub-Kelvin temperatures. Although "weak", these interactions dominate the physics at low temperatures and can give rise to completely different (classically unexpected) reaction outcomes.

I will describe our apparatus that is designed to cool and trap multiple species of atoms, ions and molecules simultaneously. We employ the standard techniques of laser-cooling to cool and trap lithium and cesium atoms at temperatures below 1 mK. We study collisions between ultracold lithium and cesium atoms and show that collisional loss rates can be controlled by controlling the quantum state of the colliding atoms. We also study collisions between neutral ultracold atoms and singly charged ions. We show sympathetic cooling of ions by the ultracold atoms. I will discuss our ongoing efforts towards making ultracold polar molecules by associating ultracold atoms. Finally, I will briefly talk about an unrelated work on high resolution Doppler-free two-photon spectroscopy where we observe a quantum interference phenomenon for the first time.

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Glycosylation and Glycodiversification through Sustainable Mode

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Carbohydrates, the vital endogenous biomolecules, found mostly in conjugation with lipids (to form glycolipids) and proteins (to form glycoproteins), are composed of various monosaccharide units linked together through *O*-glycosidic linkages. They serve for the storage of energy (starch and glycogen) and form much of the structural framework of cells and tissues (cellulose and chitin). Carbohydrate processing enzymes are responsible for making and breaking the chief glycosidic linkage and have been implicated in controlling diseases like influenza infection, cancer, AIDS, Gaucher's disease and diabetes.[1] Therefore, the formation of glycosidic bonds is one of the important aspects of carbohydrate chemistry. Anomeric trichloroacetimidates are the most effective and commonly used glycosyl donor in chemical synthesis for glycosylation reactions.[2] In recent years, many new benchtop stable and readily available glycosyl donors have been introduced in the literature.[3-4] However, still there is a large demand from organic chemists to find new glycosyl donors which favor the smooth *O*-glycoside bond formation in high anomeric selectivity. This talk will summarize the conceptually novel approach used in stereoselective glycoside bond formation and glycodiversifications.[5] The mechanistic details followed by the different catalysts and further application of these methods in the synthesis of complex saccharides will be also discussed.

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Construction of Multifunctional Rotaxanes and Rotaxane-Peptide Conjugates for Targeted Imaging

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The design of NIR fluorescent (650–1000 nm) probes is important for super-resolution imaging because of their deep tissue infiltration, minimal autofluorescence, and weak background noise. I'll demonstrate how to synthesize NIR fluorescent rotaxanes in solid phase on resin.[1] NIR rotaxane-peptide conjugates with dual-targeting functionality will be emphasized for active targeting of live cancer cells, subsequently selective staining of lysosomes and mitochondria.[2] Single imaging methods like USG, CT, PET, SPECT, MRI, and fluorescence imaging have garnered a lot of interest in biomedical research and clinical diagnostics. Each imaging method has inherent benefits and drawbacks regarding sensitivity, penetration depths, resolution, and the possibility of radiation exposure (for CT) and radioactive material hazards (for PET/SPECT). NIR fluorescence (NIRFL) has a quick response and great molecular sensitivity. However, NIRFL imaging has inherent drawbacks, such as its incapacity to provide 3D anatomical data. MRI, on the other hand, has a greater spatiotemporal resolution than other imaging techniques and allows for unlimited penetration depth and 3D tomography of soft tissues. However, MRI has low detection sensitivity and is unable to track molecular events. A single imaging technique cannot provide complete information and is unlikely to provide all the requirements to treat a diagnostic problem. The integration of imaging tools like PET/CT and PET/MRI is designed into commercial imaging instruments that are being used in clinical settings. Since MRI and NIRFL don't contain radioactive chemicals or dangerous ionizing radiation, their combination is beneficial. However, a significant drawback is that NIR dyes often undergo quenching when capped onto a superparamagnetic Fe_3O_4 NP-based MR contrast agent. We found that quenching and bleaching of the dye inside the live cells, along with the dye aggregation problems, could be mitigated by interlocking the NIR probe inside a macrocycle to create rotaxanes that are capped on the Fe_3O_4 NPs.[3] Water-soluble, noncytotoxic rotaxane-capped Fe_3O_4 NPs with a high relaxation rate (r_2) of 180.7 mM^{-1} s^{-1} are employed for live-cell mitochondria-targeted NIR fluorescence imaging in amalgamation with T_2-weighted MRI.[3] The main problem with confocal laser scanning microscopy is that mitochondrial cristae cannot be resolved due to its resolution limit of about 200 nm. One popular imaging method that has the potential to revolutionize modern bioimaging is stimulated emission depletion (STED) super-resolved fluorescence microscopy. We will demonstrate the creation of a smart NIR fluorescent rotaxane-peptide bioconjugate that can be applied to targeted live cancer cells submitochondrial STED and multimodal imaging.[4,5]

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Organic Stress: A Tool for Chemical Synthesis

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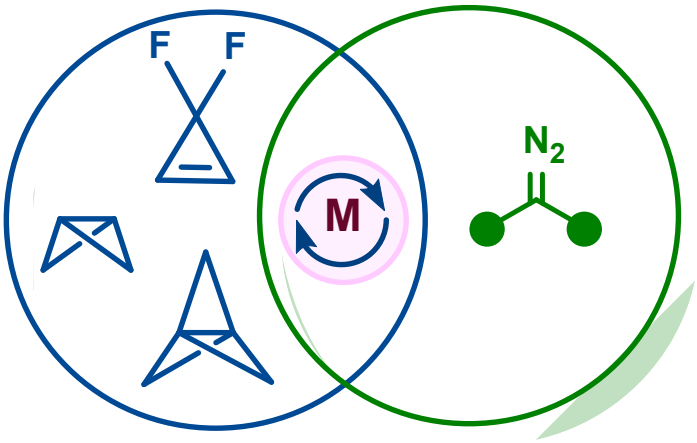
Ring-strain in organic molecules is a powerful driving force that promotes reactivity through strain-release, allowing the facile construction of a myriad of useful scaffolds via ring-opening or ring-expansion reactions. Carbene chemistry has been widely studied, and numerous applications in organic synthesis such as X–H (X = C, Si, N, O, etc.) insertions, cyclopropanations, ylide formations, and 1,2-migrations. Due to their high reactivity, carbenes are also ideal for initiating a cascade sequence, leading to rapid generation of structural complexity. We have merged strain-release and metal-carbene chemistry to unlock new strategies for organic synthesis. In this lecture, I will first discuss a copper-catalyzed highly diastereoselective strain-release [2,3]-sigmatropic rearrangement.[1] Then, I will present how we utilized the ring strain in [1.1.1]propellane to access copper-carbenes for [2,3]-sigmatropic rearrangement.[2] At the end, I will focus on rhodium-catalyzed strain-enabled stereoselective synthesis of skipped dienes.[3]



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Self-assembled Rotaxane with Redox-active Stopper

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Abstract:

Dynamic Stereochemistry of Interlocked molecules is of fundamental interest as it inspires the design of artificial systems of definitive functions/ motions.[1] This led to Nobel Prize-winning discoveries of molecular rotors, shafts, and machines that depicted controllable movements and relative motions of molecular components that impact the properties of robust architectures.[2] These inter-connected molecular assemblies exert a symphony of *non-covalent interactions,* triggering the molecular motion from the sub-nanometre level to the macroscopic scale. Among the various classes of interlocked molecules, our prime interest is **Rotaxane**,[3-5] which consists of two components: i) a rod-shaped molecule with bulky stopper units termed **Axel** (dumbbell shape) and ii) a **wheel**-shaped macrocycle that is mechanically interlocked (Figure 1) through non-covalent interactions like halogen bonding[3, 5-7], π - π interaction,[3] electrostatic interactions, etc.[8, 9] In this work, we demonstrate a *self-assembled* rotaxane embedded with a redox-active ligand/ Lindqvist polyoxovanadates as the terminal to induce the redox properties. Electrostatic repulsion around the terminals forces the wheel inside the interlocked scaffold. Furthermore, the presence of the electron donor centers at the terminal enables it to get anchored on the oxygen atom deficient surface of the Lindqvist polyoxovanadates, which have never been used as *stoppers,* and these can leverage the redox activity/ stability on the stopper itself. The size and shape of the POVs match well with the conventional stoppers, satisfying its key aspect (not to allow de-threading), but strongly differs from the architecture of the *redox-in-active* bulky stopper ends.

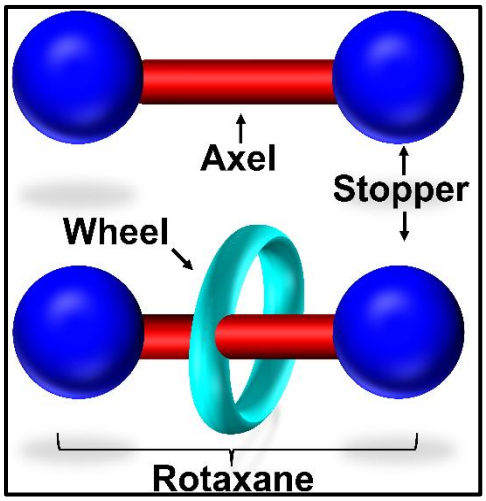

Figure 1: Cartoon depiction of an axel, wheel and Rotaxane.

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Cold Chemistry: Investigation of atom – molecule interactions at cold conditions and probing quantum effects in the interaction

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Cold chemistry is the investigation of interactions of atoms and molecules at near-absolute-zero temperatures, few-Kelvin to milli-Kelvin range. Cold conditions enable the study of chemical reactions with full control over the reaction parameters. Colliding particles at these temperatures reveals quantum nature of interaction between any atoms or molecules; quantum effects such as resonances become observable and lead to sharp increase in collision cross section. Such unambiguous identification of resonances enables subtle features on the underlying potential energy surfaces to be probed, enabling us to get the first look at what exactly happens during a chemical reaction. Cold chemistry is also important for the understanding the rich gas phase chemistry occurring at the interstellar medium and the upper atmosphere, where reactions are expected to proceed through quantum mechanisms, unlike at room temperatures. Therefore, such experimental measurements enable the accuracy of high-level theoretical calculations to be assessed and the validity of such models of chemical reactivity to be tested. In the talk, I will show the results of an experiment, where a merged beam method is used in combination with velocity map imaging technique to probe the dynamics of $He^* - D_2$ collisions in the range 1.0 to 50.0 K experimentally. In our studies, we distinguish between two mechanisms of formation of resonances by comparing the elastic and Penning ionization cross sections (this work has been recently published in *Nat. Chem.*, **13**, 94, 2021). In this work we show two different resonances – shape and orbiting in the interaction of He^* and D_2. Our results show resonances at 2.0, 4.0 and 8.0 K in the elastic scattering cross section whereas only the 2.0 K resonance is visible in the Penning ionization spectra (fig. 1). Shape resonances appear as sharp peaks in both processes whereas orbiting resonances only appear in the elastic cross section since the probability of finding particles at short separation, where ionization takes place, is small. In this work, we report the first experimental identification of these two mechanisms. I will also discuss my research interest.

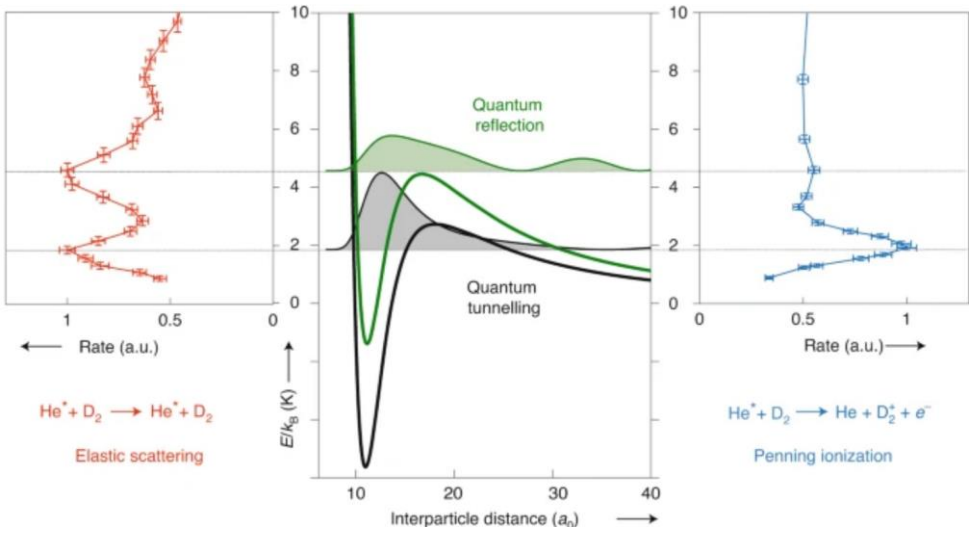

Fig. 1 Relative rate constant of He^*-D_2 elastic collisions (left), and Penning ionization process for the same system (right).

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Mechanistic insight of the electro-reduction of nitrate to ammonia on metal-oxide electrocatalyst

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Abstract: Electrocatalytic nitrate reduction reaction (eNO_3RR) to produce green ammonia is not only a sustainable solution to bypass the energy-intensive Haber-Bosch process but also thermodynamically challenging due to the requirement of sequential multielectron ($8e^-$) and proton ($9H^+$) transfers. The selective reduction of nitrate to ammonia proceeds via the formation of multiple reaction intermediates like $[NO_2]^-$, [NO], and $[NH_2OH]$. The rate-determining step of eNOR is the formation of $[NO_2]^-$, and the selectivity toward NH_3 (over NO_2, NH_2OH, N_2) formation is controlled by the optimum adsorption of the $[NO_2]^-$ intermediate to the catalyst surface. In our recent studies, metal-oxide nanoparticles such as FeO(OH) and Mo_7 cluster-protected CeO_2 nanoparticles were chosen as electrocatalysts to perform selective eNO_3RR to produce NH_3.[1-2] Detailed electrochemical studies were conducted to understand the electrochemical rate constant. ^{15}N- and D-labeling and in-situ vibrational spectroscopic studies were conducted to track some reactive intermediates of eNO_3RR to validate the reaction mechanism on the metal-oxide surface (Figure 1). In my talk, I will briefly present these recent findings.

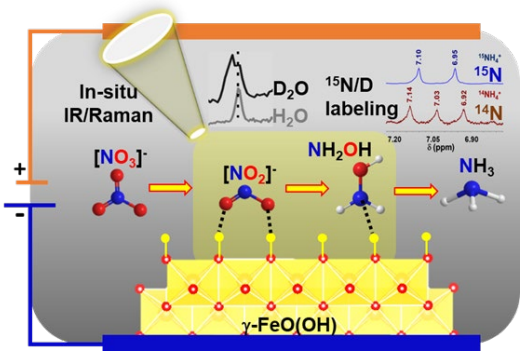

Figure 1. Electrocatalytic nitrate reduction on FeO(OH) and in-situ tracking of the reaction intermediate

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Excited-state Redox Bimodality of Indigo Behaving as both Super-oxidant and -Reductant

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Indigo is an extremely popular molecule in dye industry, however, its use in photochemical transformations is surprisingly scarce. We present its photocatalytic activity over an unusually wide excited-state redox window. We showcase that the dye molecule exhibits bimodality and proves itself as a simultaneous super-reductant and -oxidant, spanning a massive redox window of 5.98 V. This extreme bimodal behavior in indigo originates from the viability of two electron redox processes on the parent architecture. In comparison, major popular photocatalysts (PC) usually can accept or donate only one electron, limiting the span of its bimodal redox window significantly. In the presence of KO^tBu and white light irradiation, indigo is converted to its tetraanionic form, Ind^{4-} which displays its super-reducing power to an extent of -3.6 V vs SCE. Such an in situ-generated species has been separately synthesized and the reductive prowess of the PC has been examined for a wide array of reactions which starts with a reductive cleavage of the C-Cl bonds. On the contrary, the super-oxidant behavior of indigo has been explored in the presence of a mild oxidant and blue light irradiation, generating dehydroindigo. The strong oxidizing capability of the PC has been utilized for ipso-substitution of aryl fluorides with a series of nitrogen-based nucleophile.

Probing and tuning the chemical reactions at a single molecular level.

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The traditional chemical analysis techniques for probing the reaction kinetics, such as Mass spectrometry, NMR, IR, and UV-Vis spectroscopy, have certain detection limits associated with them (i.e. in the order of few ppm). It is not trivial to further increase the detection limit of these traditional techniques to a single molecule level. In this context, we envisage that the highly sensitive MCBJ technique can become a promising platform for reaction detection studies with the lowest detection boundary, i.e., single-molecule level.[1] To achieve this goal, two immediate strategies one had to develop were finding a way to carry out the reaction within the MCBJ setup and correlating the data (conductance-distance traces) collected corresponding to the molecular junction to the in-situ chemical reaction. The conductance-distance traces obtained after the measurement serve as a fingerprint for the molecular system under observation, and the continuous measurement of conductance-distance traces of the molecular junction throughout the chemical reaction serves as a matrix to extract the rate information. Then, the precise data analysis methodology was developed for getting the presence and proportion of different molecular species (reactant/product/intermediate) inside the reaction mixture from the bulk data using machine learning tools. Using this framework, we have tried to probe various chemical reactions at a single molecular level. In my talk, I will give a brief overview of different chemical reactions that we are probing at single molecular level.

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Role of Magnesium in RNA Folding

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The folding of RNA is highly sensitive to its surrounding counter-ion environment. Among different prevalent metal ions in cellular composition, the physiological concentration of magnesium (Mg^{2+}) (~1-2 mM), in addition to a monovalent salt (≥ 100 mM), is often found critical in stabilizing an RNA fold. In this seminar, I'll first elucidate our recent characterization of RNA ion-atmosphere using explicit solvent molecular dynamics simulations.[1] The simulations supported by experiments show that based on the direct and indirect coordination between Mg^{2+} and RNA, these ionic species can be classified into (i) inner sphere ions/chelated, (ii) outer sphere ions, and (iii) diffuse ions. However, understanding the specific functional roles of these ion-atmospheric components in RNA folding remains challenging through classical simulation methods due to long-time scale related computational sampling issues. Addressing these challenges, we have developed a structure-based model of RNA integrating extended Debye-Hückel and Manning counter-ion condensation theory of polyelectrolyte[4]. In this model, we treat high concentration of K^+ monovalent salt buffer implicitly and to assess specific RNA-Mg^{2+} correlation, we treat all-atoms of RNA and Mg^{2+}, explicitly.[2,3]. I'll discuss our recent advancement where we have also introduced the dynamic ion exchange phenomena between inner and outer-sphere Mg^{2+}, into the structure-based model. All these new advancements of simulation method now enable us to explore and predict Mg^{2+}-induced large-scale structural dynamics and folding/functional free energy landscape of RNA.[3]

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Two-dimensional Electronic Spectroscopy: Do Vibronic Couplings Survive in Large Photosynthetic Aggregates at Room Temperature?

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Abstract

Research on natural photosynthetic proteins so far has demonstrated the existence of delocalized states at cryogenic temperatures arising from a mixing of electronic and vibrational degrees of freedom. Theoretical and (limited) experimental evidence suggests that such design principles crucially rely on energetic disorder and a dense low-frequency Raman active spectrum in the Q bands of chlorophylls. The resulting energy funnels are highly non-adiabatic and may be crucial to photosynthetic efficiency. Do such delocalized states survive in large aggregates at room temperature is an open question. The hot debate[1,2] around the functional role of vibronic couplings in photosynthesis revolves around this fundamental question. Parallel research on artificial light harvesting systems has largely focused on approaches based on cyanine molecules to achieve either self-assembled nanotubes or DNA templates with precise control over distance and relative orientations. It is not clear whether cyanine-based templates allow us to mimic the photosynthetic design principles because Huang-Rhys factors, vibrational frequencies and electronic structure of cyanine dyes are all significantly different from chlorophylls.

Two-dimensional electronic spectroscopy (2DES) provides femtosecond (fs) temporal resolution along multiple spectral dimensions – excitation, emission and coherence axes, and has revolutionized our understanding of natural phenomena ranging from internal conversion that triggers mammalian vision, energy and charge transfer in photosynthesis, exciton dissociation in photovoltaics and layered materials. We have developed[3,4] a 2DES spectrometer that provides sub-10 fs temporal resolution over a >100 nm bandwidth and provides throughput and sensitivity higher than the current state-of-the art approaches. In this work we apply our spectrometer to investigate self-assembled porphyrin nanotubes whose overlapping vibrational-electronic Q bands closely resemble those found in photosynthetic proteins. By spectrally decongesting such bands through 2DES and selectively probing the mixed Qx-Qy states through the use of polarization control, we find that vibronically mixed Qx-Qy states indeed survive in large aggregates at room temperature and dictate ultrafast intraband population relaxation. Our work carries direct implications for the debate around the functional role of vibronic couplings in photosynthetic energy/charge transfer and argues that artificial light harvesting systems based on chlorophyll-like molecules may be the ideal templates for leveraging the design principles of natural light harvesting.

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Interfacial dipole at metal-water junction: How important is the water contribution?

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Metal-water interface plays a critical role in several heterogeneous processes, with or without applied potential. In this work we employ the framework of partially occupied wannier functions to assign the 'position' of the valence electrons of water molecules near an uncharged gold surface and compute the dipole moment of individual water molecules within the framework of ab initio molecular dynamics. The ensuing analysis suggests that the gold surface strongly polarize the lone pair of electrons of the water molecules in close proximity to the interface and pointing towards the surface. Consequently, the total electronic interfacial dipole has a significant contribution from the water dipoles in the near vicinity.

InAdvanCS 2025 SCS Annual Symposium [21 Feb 2025]

Student presentation schedule (5 mins each)

Sl. No.	Student Speaker	Title
1	*Souvik Dinda*	Proton-Coupled Electron Transfer between a Pendant Thiol and a Ferrous Dioxygen Adduct
2	*Kamal Hossain*	Thiocarboxylate and Acid Chloride Mediated Generation of Nitric Oxide from a Dinickel(II)-bis(ONO) Complex Involves the Formation of Perthionitrite and O-nitrosyl Carboxylate
3	*Anuj Kr Ray*	Predicting Spin State Gaps of Transition Metal Complexes Using Electronic Structure Calculation-Based Descriptors
4	*Ankita Das*	Tuning the Conditional Mechanochemical Reactivity of Molecules.
5	*Rohon Mitra*	Metamorphism and IDP Folding: Insights from a Multiple Native States Model
6	*Supriyo Santra*	Deciphering the mechanism of singlet fission in carotenoids
7	*Anirban Panua*	s /p-(non/anti) Aromatic singly and doubly N-confused tetra pyrrolic(heterocyclic) macrocycles
8	*Ishita Roy*	Palladium catalyzed selective C-H functionalization utilizing aldehyde autoxidation
9	*Nabin Parui*	Synthesis of Cyclohepta[b]indoles and Cyclohepta[b]indole-Indoline Conjugates
10	*Anushree Dutta*	Simulation and Design of Cold Collision Apparatus to study reaction dynamics at low temperature.
11	*Nabanita Roy*	Designing a vehicle-free anti-bacterial topical hydrogel from Fmoc-diphenylalanine
12	*Soumya Mondal*	Photocatalytic Generation of Phenacyl Synthon from α, β- Unsaturated Acids for C-C/Het Cross Coupling
13	*Sujan Paul*	Journey towards Stereoselective Total Synthesis of Nonribosomal Cyclic Pentapeptide Nemamide A & Euglenatide D-E
14	*Saikat Hazra*	Ortho-Para Conversion for $H^+ + H_2$ Collision in Low Temperature: A Fully Closed Coupled Time Dependent Wave Packet Study
15	*Chinmay Dey*	Copper-Aβ and Cytochrome c: A Potential Janus in Alzheimer's Disease
16	*Arghyadip Bhowmik*	Influence of Carbene Carbanion Equilibrium for tris-(2-pyridylthio)methanido Ligand on the Dioxygen Reactivity of Biomimetic Iron(II)-Benzilate Complexes
17	*Mahuya Kar*	Micellization and Demicellization of Multi-Responsive Poly(2-oxazoline) Azo-bridged Graft Copolymers