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Chemistry Interfacing with Biology and Physics

27-28 January 2017

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Chemistry Interfacing with Biology and Physics (CIBP)

27-28 January 2017

Abstract Book

Organized by

Indian Institute of Science Education and Research Kolkata

Preface

IISER Kolkata has emerged to be an institute of scientific excellence in India. In continuing its pursuit in science this year it is celebrating 10 years of excellence. This conference "Chemistry Interfacing with Biology and Physics (CIBP)" is part of this celebration and is devoted to recent advances and new trends in chemistry which reaches out to encompass various challenges in physics and biology research in an integrated manner. This includes supramolecular chemistry, organometallic chemistry, bio-inspired coordination chemistry, design of new functional materials, nano-sciences of metal and its complexes, surface chemistry and other emerging topics in chemistry. This conference is intended to be highly multidisciplinary in nature, which will bring together scientists working in areas of chemistry, physics, biology, medicine and nano materials.

Director's Message

The strength of IISER Kolkata (IISER-K) is derived from its talented students, faculty, state-of-the-art research facilities, and flexibility of academic program. An important aspect of IISER-K is its interdisciplinary character, as modern science education and research focus on broader perspectives. Keeping this in mind, IISER-K offers BS-MS (5-yr. Integrated Masters) program, involving two years of compulsory exposure to all the science disciplines to study Physics, Chemistry, Mathematics and Statistics, Biology, and Earth and Planetary Sciences along with introduction to Computer Programming and Electronics, followed by two years of study in a 'major' discipline, and finally one year devoted to research leading to a Masters' thesis. In addition to BS-MS program, IISER-K also has post-BSc Integrated PhD program, as well as post-MSc PhD program. PhD programs are specifically focused on cutting-edge research. Notably, all pre-doctoral students receive stipends to meet their academic expenses. We are very happy that the first few batches of BS-MS alumni of IISER-K have booked their places in some of world's best research institutes for advanced studies. We are sure a similar trend will continue. It is a matter of great satisfaction that faculty members are publishing their research papers in journals of international repute, based on work done at IISER-K. Some of our young faculty members have excelled in research and have been recognized with national and international fellowships/awards. Apart from engaging in scientific activities, students and faculty of IISER-K are also involved in various social and outreach activities. The academic activities of IISER-K are supported by sincere staff members. We all – the members of IISER-K family-feel proud of being a part of this budding institution. To conclude, for inquisitive young minds looking for a platform for experiencing a fine blend of quality teaching with world-class research in basic science, IISER-K is one of the best institutions to reckon with.

I wish a great success!

Professor R. N. Mukherjee

Director

Indian Institute of Science Education and Research (IISER) Kolkata

Message: DCS Chairperson

The Indian Institute of Science Education and Research Kolkata was founded in 2006 by the Ministry of Human Resource Development (MHRD), Government of India and one of the first departments to be established was the Department of Chemical Sciences (DCS). From the beginning, the Department has incarnated the Institute's mission of excellence in both research and teaching. The DCS has appreciable strength in the core areas of physical, organic and inorganic chemistry as well as in interdisciplinary research areas at the boundaries with physics, biology, earth science and materials science. An extremely wide range of state-of-the-art instrumentations are available in different research groups to carry out the DCS research activity.

This conference is devoted to recent advances and new trends in chemistry which reaches out to encompass various challenges in physics and biology research in an integrated fashion using the knowledge of the three subjects. This includes supramolecular chemistry, organometallic chemistry, bio inspired coordination chemistry, design of new functional materials, nano-sciences of metal and metal complexes, surface chemistry and other emerging topics in chemistry. The conference is highly multidisciplinary and therefore will bring together scientists working in areas of chemistry, physics, biology, medicine and nano-materials.

I am looking forward to sharing a most pleasant, interesting and fruitful conference.

Pradip Kr. Ghorai

Scientific Programme

27 January 2017		
7:30 AM - 8:30 AM	:	*Registration*
8:00 AM - 9:00 AM	:	*Breakfast*
9:00 AM - 9:30 AM	:	*Inauguration*
1st Session	**:**	***Chemical Biology (Chair: Dr. C. Malla Reddy)***
9:30 AM - 10:00 AM	:	Talk 1: Prof. Sandeep Verma, IIT Kanpur
10:00 AM - 10:30 AM	:	Talk 2: Prof. Srinivas Hotha, IISER Pune
10:30 AM - 11:00 AM	:	*Tea Break*
2nd Session	**:**	***Chemical and Materials Physics (Chair: Dr. P. Mandal)***
11:00 AM - 11:30 AM	:	Talk 3: Dr. Jyotishman Dasgupta, TIFR, Mumbai
11:30 AM - 12:00 PM	:	Talk 4: Dr. Arindam Chowdhury, IIT Bombay
12:00 PM - 12:30 PM	:	Talk 5: Dr. Anshu Pandey, IISc, Bengaluru
12:30 PM - 1:00 PM	:	Talk 6: Dr. Kanishka Biswas, JNCASR, Bengaluru
1:00 PM - 2:00 PM	:	*Lunch*
2:00 PM - 3:00 PM	:	Poster Session
3rd Session	**:**	***Biological Chemistry (Chair: Dr. Rahul Das)***
3:00 PM - 3:30 PM	:	Talk 7: Prof. Gautam Basu, Bose Institute, Kolkata
3:30 PM - 4:00 PM	:	Talk 8: Dr. Ruchi Anand, IIT Bombay
4:00PM - 4:30 PM	:	*Tea Break*
4:30 PM - 5:00 PM	:	Talk 9: Prof. Siddhartha Roy, Bose Institute, Kolkata
5:00 PM - 5:30 PM	:	Talk 10: Dr. Mahesh Hariharan, IISER Thiruvananthapuram
7:30 PM - 9:30 PM	:	*Conference Dinner*

28 January 2017		
8:00 AM - 9:00 AM	:	*Breakfast*
1st Session	**:**	***Chemical Biology (Chair: Prof. R N Mukherjee)***
9:30 AM - 10:00 AM	:	Talk 11: Prof. Santanu Bhattacharya, IACS, Kolkata
10:00 AM - 10:30 AM	:	Talk 12: Prof. Vibha Tandon, JNU, New Delhi
10:30 AM - 11:00 AM	:	*Tea Break*
2nd Session	**:**	***Synthesis for Drug Discovery (Chair: Dr. Debasis Haldar)***
11:00 AM - 11:30 AM	:	Talk 13: Dr. Manmohan Kapur, IISER Bhopal
11:30 AM - 12:00 PM	:	Talk 14:Dr. Harinath Chakrapani, IISER Pune
12:00 PM - 12:30 PM	:	Talk 15: Dr. Jyotirmoyee Dash, IACS, Kolkata
12:30 PM - 1:00 PM	:	Talk 16: Dr. S. V. Rama Sastry, IISER Mohali
1:00 PM - 2:00 PM	:	*Lunch*
2:00 PM - 3:00 PM	:	Poster Session
3rd Session	**:**	***Medicinal Inorganic Chemistry (Chair: Dr. Supratim Datta)***
3:00 PM - 3:30 PM	:	Talk 17: Prof. A. R. Chakravarty, IISc, Bengaluru
3:30 PM - 4:00 PM	:	Talk 18: Dr. Amitava Das, CSMCRI, Bhavnagar
4:00 PM - 4:15 PM	:	Vote of thanks
4:15 PM - 5:00 PM	:	*High Tea*

INVITED LECTURES

Nucleobase Functionalization for Metal Coordination: Material and Biological Applications

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We will describe design strategies for modified adenine nucleobase derivatives to construct metal-mediated discrete complexes, ring expanded purine skeletons, linear and catenated coordination polymers, shape-selective MOFs, and purine-capped nanoparticles, with wide-ranging applications from gas and solvent adsorption to bioimaging agents and anticancer metallodrugs.1 such strategies rely on rich chemistry of purine and pyrimidine derivatives, versatile coordination behavior, ability to bind a host of metal ions, which could be further tuned by the introduction of additional functionalities, and their inherent propensity to hydrogen bond and exhibit π-π interactions.[2]

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1. (a) Inorg. Chem.,**2016**, *55,* 7041-7050; (b) *Sci. Rep.,* **2016** (DOI:10.1038/srep24499); (c) ChemPlusChem., **2016**, *81*, 1266-1271; (d)*Chem. Eur. J.* **2014**, 20, 12262-12268.
2. Acc. Chem. Res.,2010, *43,* 79-91.

‘Gold’en Era in the Synthesis of Mycobacterial Saccharides

Srinivas Hotha and All the Member of the Chemical Glycosylation Laboratory

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Tuberculosis is caused by Mycobacterium tuberculosis (Mtb) was first discovered in 1882 by Robert Koch and observed that Mtb has a thick and waxy coating on its cell surface giving a tough barrier for antibiotics to enter for eventual killing. Decades later, Brennan has unravelled the complete cell wall structure of Mtb to find that the cell surface contains some unusual saccharides in furanosyl form which are otherwise not observed in other bacterial mammalian species. Indeed, several first line drugs which are currently administered for patients suffering from tuberculosis are noticed to inhibit the biosynthesis of cell wall. It is in this context, the synthesis of cell wall fragments of Mtb gained momentum over the past two decades; many groups have hit upon synthesizing the truncated epitopes of Mtb cell wall.

Our group discovered the use of gold(III) chemistry for the glycosidation using alkynalated sugars as glycosyl donors [1-4]. Several glycopyranosyl donors had undergone gold-catalyzed glycosidation to synthesize glycomimetics, glycopolyacrylates, glycopolyacrylamides, glycopolypeptides etc. which are otherwise very difficult to synthesize.

Over the last five years, the focus of the group shifted to the synthesis of furanosides and developed practical methods for their synthesis in a stereoselective fashion [2,4]. Over the last couple of years, the assembly of large oligofuranosides with a goal towards developing a vaccine for tuberculosis using the unique glycolipid of the cell surface of Mtb was investigated [3]. We have successfully synthesized large oligomeric structures of arabinogalactan and lipoarabinomannan portions of the Mtb cell wall. Results of this study will be presented in the seminar [5,6].

Acknowledgements: DST-New Delhi and CEFIPRA-New Delhi for the financial assistance.

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Tracking the Fate of Singlet Excitons in Conjugated Organic Materials: *Relaxation and Fission*

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One of the major challenges in developing robust photon-conversion technologies from organic materials is the ability to precisely manoeuvre or direct photo-generated excitons at device interfaces. [1] The translational diffusion of excitons through an organic backbone critically depends on the complex interplay of its excess energy and the intervening material morphology. Conventionally the fate of singlet excitons is tracked using time-resolved absorption or emission spectroscopies which are inherently insensitive to structural changes associated with exciton diffusion or its dissociation. [2] Through this talk, I will demonstrate that femtosecond time-resolved Raman spectroscopy can provide structural snapshots of excitonic relaxation and its partial dissociation in the manifold of the singlet states. The obtained molecular view of relaxation reaction coordinate(s) does provide significant clues to optimize the polymer backbone for efficient charge generation. I will also highlight our efforts to tune material morphology to engineer singlet exciton fission in conjugated molecules which have the correct Singlet-Triplet ($E_S \sim 2E_T$) [3] energy gap. Finally, I will conclude by detailing a coherent perspective to exciton dynamics necessary for building an energy efficient organic photovoltaic device.

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Spatiotemporal Heterogeneity in Optoelectronic Behaviors of Perovskite Micro and Nano-Crystals

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Hybrid (organic-inorganic) perovskites have been in recent limelight for tremendous progress in light to energy conversion efficiencies as well as usage as LED displays due to a wide range of color tunability, although there are some stability issues that need to be addressed. Methyl ammonium lead iodide (MAPbI3) and its analogues possess several relevant properties, such as high extinction coefficient and carrier diffusion length, which make them suitable for photovoltaic applications. With the intention to enhance stability, it was recently demonstrated that incorporation of pseudo-halide molecular anions (SCN-) as dopants in the MAPbI3 severely affects the ensemble optoelectronic properties, resulting in a remarkable enhancement of photoluminescence (PL) quantum yield along with slight lowering in the optical band-gap. To understand this, as well as investigate microscopic uniformity in photoemission properties, PL microscopy was performed on SCN-doped MAPBI3 crystals under ambient conditions. [1] Our results clearly shows spatially heterogeneous, site specific emission from individual MAPbI3-x(SCN)x microcrystals, where grain boundaries most often exhibit extremely high radiative recombination efficiency as compared to the interior regions. Spatially-resolved PL spectroscopy and lifetime-imaging measurements also reveal considerable non-uniformity in the local electronic structure and carrier recombination dynamics amongst various nanodomains within the interior regions/grain-boundaries. Intriguingly, temporal instability, i.e., dynamical fluctuations in luminescence from local nanodomains was observed within individual microcrystals, reminiscent of PL intermittency (or blinking) known to occur for single semiconductor nanocrystals (quantum-dots). The possible origins of such spatiotemporal heterogeneity will be discussed in context of similar observations in other perovskites. I will also discuss unusually (suppressed) luminescence blinking dynamics and photo-triggered delayed emission in highly luminescent CsPbBr3 nanocrystals which may have potential applications stable single-photon sources.

References:

1. A. Halder, R. Chulliyil, A.S. Subbiah, T, Khan, S. Chattoraj, A. Chowdhury, S.K. Sarkar, The Journal of Physical Chemistry Letters, 2015, 6, 3483-3489

Chemistry with Bigger Atoms

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We demonstrate the formation of ground state charge transfer states in a binary quantum dot (QD) mixture. Charge is observed to reside in quantum confined states of one of the participating QDs. These interactions lead to materials that may be regarded as the nanoscale analog of an ionic solid. The process by which these materials form has interesting parallels to chemical reactions in conventional chemistry. Conventional solids are prepared from building blocks that are conceptually no larger than a hundred atoms that are held together by interactions that extend to sub-nanometric lengths. The QD compounds prepared by us, in contrast are held together by interactions that appear to be chemical bonds, only scaled up in strength and length scale by over an order of magnitude. We will discuss interesting physical phenomena that arise in these materials and also describe the origins of stoichiometry and other atom-like properties in QDs.

Origin of Ultra-Low Thermal Conductivity in Complex Chalcogenides: Effect of Intergrowth Nanostructure, Lone Pair and Rattling

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Thermoelectric materials can directly and reversibly convert waste heat into electrical energy, and will play a significant role in future energy management. One of the fundamental challenges in developing high-performance thermoelectric materials has been to achieve low lattice thermal conductivity (K_L). The exploration of new materials with intrinsically low K_L along with a microscopic understanding of the underlying correlations among bonding, lattice dynamics and phonon transport is fundamentally important towards designing promising thermoelectric materials. The origin of lattice anharmonicity and the ensuing ultralow K_L in the I-V-VI_2 chalcogenides such as $AgSbSe_2$, $AgBiSe_2$, $AgBiS_2$ and AgBiSeS has been traced to the electrostatic repulsion between the stereochemically active ns^2 lone pair of group V cation and the valence ρ-orbital of group VI anion.[1] InTe [i.e. $In^+In^{3+}Te_2$], a mixed valent compound, exhibit an ultralow K_L, which manifests an intrinsic bonding asymmetry with coexistent covalent and ionic substructures.[2] The phonon dispersion of InTe exhibits, in addition to low-energy flat branches, weak instabilities associated with the rattling vibrations of In^+ atoms along the columnar ionic substructure. These weakly unstable phonons originate from the $5s^2$ lone pairs of adjacent In^+ atoms and are strongly anharmonic, which scatter the heat-carrying acoustic phonons through phonon-phonon interactions. AgCuS exhibits ultra low K_L and it composed of softly coupled cationic and anionic substructures, and undergoes a transition to a superionic phase with changes in the substructure of mobile ions with temperatures.[3] Electronic density of states and phonon dispersion reveal that the rigid sulphur sub-lattice is primarily responsible for the electronic charge transport, whereas soft vibrations and mobility of Ag/Cu ions are responsible for the ultra-low thermal conductivity. Formation of layered intergrowth nanostructures in solid matrix by kinetic matrix encapsulation can also lead to ultralow K_L.[4]

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Simple Physical Models for Complex Biological Processes

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Interaction between two protein molecules or interaction between a small molecule and a large protein drive a plethora of biological functions. However, to be biologically relevant, these interactions must be specific. In other words, the 'right' pair should interact but not the 'wrong' pair. Therefore, evolution must have incorporated both 'positive' and 'negative' design in the biologically relevant molecule-molecule interaction—the positive design optimizing the interactions between two cognate partners while the negative design keeping two non-cognate partners away from each other. I will use two examples—the case of discrimination between guanine and adenine by proteins [1], and, the case of protein-protein association kinetics [2,3]—to show how simple electrostatic models can explain experimental data relating to both the phenomenon. Further, because the models are very simple although they explain complex processes, this is an example of Ockham's razor, a philosophy often used in science that the simplest among more complex hypothesis should be chosen.

Structure Guided Design of Aromatic Biosensors

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One of the major sources of environmental pollution from various industrial sources is toxic aromatic pollutants like phenol, benzene and their derivatives (chlorophenols, cresols, xylenes, xylenolsetc). Many of them pose grave threat as they are persistent in the environment and are carcinogenic and embryotoxic in nature and their exposure, even in small quantities can be lethal. Due to their small size and limited chemical versatility it is extremely challenging to employ suitable chemical strategies to develop specific sensors for these pollutants. An alternative is to exploit nature's biosensory machinery by employing transcription regulators from soil bacteria that can detect select aromatics and facilitate its catabolic degradation. However, in the absence of the crystal structure of this class of proteins the sensor development remained elusive for decades and intelligent design could not be undertaken. Here, we describe the crystal structure of the signal sensing domain of phenol regulator, MopR, from Acinetobacter calcoaceticus, in complex with phenol and its derivatives [1]. The structure helped in determination of the pocket architecture and in identifying key residues that control selectivity. It has opened doors for selective and accurate design of broad-based/specific biosensors using rational approach. Further, using structure as a template in conjunction with computational, mutagenesis and isothermal calorimetric approaches, we designed a series of selective logic-based sensors for a spectrum of aromatic compounds like catechol, xyenols, toluene, benzene etc. The biosensor activity and selectivity was quantified by constructing a longer version of the regulator, whose ATPase activity is allosterically regulated via sensor binding. Moreover, to increase the efficiency of the biosensors, we translated the targeted biosensor designs into a whole cell in vivo setup, which could detect the said pollutants with a much higher sensitivity. Based on our structure guided in vitro and in vivo biosensor designs, future efforts towards quantitative detection of these aromatic pollutants from real time contaminated environmental samples can be undertaken. This is a major stepping stone towards efficient bioremediation of target aromatic pollutants.

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A Development of Peptide-Based Synthetic Transcription Factors as Peptide Therapeutics

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Transcription factors are the primary regulators of gene expression. Many signalling pathways transduce extracellular information to alter activities of transcription factors, resulting in altered gene expression. Proteins possess ample conformational and atomic diversity to read the information present in the relatively conformationally homogeneous double-stranded DNA with high specificity. Very few classes of molecules possess enough atomic and conformational diversity to replicate that. We have thus attempted to design smaller peptide mimics of important transcription factors involved in regulation of genes important for tumor cell proliferation. We have been able to create peptide mimics of such oncogenic transcription factors as CFOS and Dlx4. In cell lines, these synthetic transcription factors rebalance the dysregulated pathways by directly regulating gene expression. The Dlx4 mimic has been shown to selective upregulate globin genes in K562 cells and human hematopoietic stem cells. Details biophysical and cellular data will be presented in the lecture.

Strategies to Reduce the Rate of Charge Recombination

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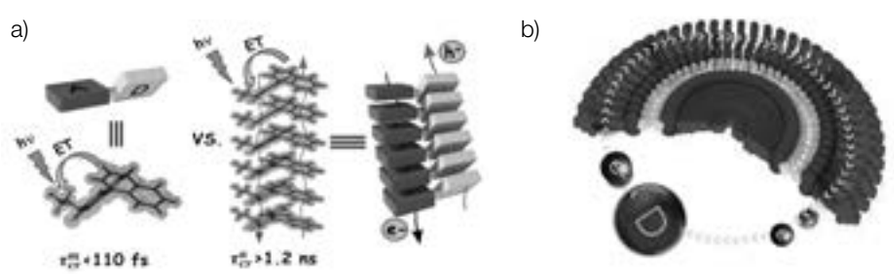
Molecules that produce charges when excited by light are useful for a variety of (bio-) organic electronic applications. To maximize the utility of these molecules, researchers work to keep the induced charges separate for as long as possible. Stacking the excitable molecules can extend the charge lifetime, but often the donor and acceptor parts of the molecule naturally alternate in the stack, which causes the charges to immediately recombine. Our group aim to minimize charge recombination [1-4] by separating the donor and acceptor portions of the molecule on different spatial planes. We have synthesized a naphthalimide-naphthalene dyad where the donor and acceptor units are twisted into different planes. The twisted monomers also assemble into a stacked tower. When illuminated by UV light, the charge separated state of the stack can last more than 1.2 ns, 10,000 times longer than in the monomeric dyad (Scheme 1). This assembly could be a novel scaffold for light harvesting, molecular electronics, or new light-induced electronic applications. As opposed to the conventional view of modulating the redox properties and/or distance between donor and acceptor, our results encourage to focus on fine-tuning of spatial organisation of the donor and acceptor chromophores to hop the charges over long distances.



Scheme 1. Representative strategies adopted in our group to spatially organize electron donors and acceptors for emergent properties.

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A Chemical Biology Approach to the Design of Bioactive and Drug Transporters

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An Odyssey of Bisbenzimidazole as Therapeutic Agent for Human Well Being

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Radiotherapy, is utilized by 80% patients as a part of their treatment to most prevalent disease like cancer. Radioprotectors protect the normal cells from the unwanted radiation damage. Since the beginning of the nuclear era, despite extensive research on the development of radioprotectors, success has been limited. We have developed a cytoprotective radioprotector DMA, having a bisbenzimidazole nucleus. Relative quantitation of gene expression of the identified proteins and their interacting partners led to the identification of NFkB inducing kinase (NIK) as one of the plausible target. Subsequently, over expression and knock down of NIK suggested that DMA affects NFkB inducing kinase mediated phosphorylation of IKKα and IKKβ both alone and in the presence of ionizing radiation. We observed 51% radioprotection in untreated cells that attenuated to 17% in siRNA NIK treated U87 cells at 24h. Further studies concluded that the co-activation of AKT/NFkB triggered by DMA, is a reason behind protection against ionizing radiation-induced apoptosis of normal cells, and this was consistent with the alteration of DNA-PKcs. Pharmacokinetic (PK) evaluations and bioavailability measurements proved superior in vivo efficacy, higher AUCs, greater residence time of DMA.

New antimicrobials are needed to combat drug resistance. One attractive strategy is to develop ligands to selectively target microbial cells over host cells. DNA minor groove binders provide useful antimicrobial agents, however, their cytotoxicity in mammalian systems limits applications. Recently, we developed bisubstituted benzimidazole with impressive DNA affinity yet surprisingly low mammalian cytotoxicity. The benzimidazole and CCCP(EPI) in combination showed synergistic effect against MDR ESKAPE bacterial strains.

New Methodologies for N-Heterocycle Synthesis via Transition-Metal Catalysis

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Short and quick assembly of highly substituted *N*-heterocycles utilizing carbon-carbon bond forming reactions via C-H functionalization have become one of the most popular research topics for synthetic chemists all over the world. [1] A variety of methods have been reported in this area. Often popular even today, low-valent metal mediated C-C bond formation reactions have been traditionally employed for the synthesis of *N*-heterocycles of biological relevance. Modern transformations based on higher-valent metal mediated C-H functionalizations provide efficient alternatives to traditional approaches. In this talk, a blend of two different approaches for the synthesis of *N*-heterocycles shall be discussed. [2]

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Small Molecule Donors of Hydrogen Sulfide (H_2S)

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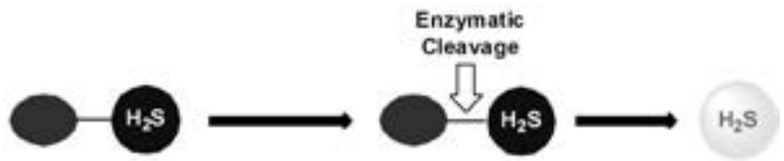
Maintenance of redox homeostasis is fundamental to cellular growth and survival. Among the emerging players in redox biology, hydrogen sulfide (H_2S), a toxic gas was long considered as an innocuous byproduct of sulfur metabolism in cells without any major roles in cells. [1] In the past two decades, the ubiquitous presence as well as diverse signaling by this gas has been reported. [1] H_2S is produced during metabolism of cysteine by cystathionine β-synthase (CBS), cystathionine γ-lyase (CSE), and 3-mercaptopyruvate sulfurtransferase (3MST) and is attributed with functions such as vasorelaxation, cardioprotection and neurotransmission. [1] Recently, it has been demonstrated that H_2S played a critical protective role during exposure of bacteria to oxidative stress as well as antibiotics. [2] The precise molecular mechanisms of cytoprotective effects of this reactive sulfur species remain to be completely elucidated. [2] Herein, we discuss our strategies [3] towards controlled generation of this reactive sulfur species within cells [4] and our progress towards identifying molecular mechanisms of action of this gas. Bis(4-nitrobenzyl)sulfanes, which are activated by a bacterial enzyme to produce H_2S were developed. Our cellular studies revealed that this novel donor was highly selective to enhance cellular H_2S in bacteria but not in mammalian cells. Using an intracellular redox biosensor, we demonstrate that H_2S protects bacteria against oxidative as well as antibiotic-induced stress by maintaining intracellular redox balance. Together, our study provides greater insight into the defence mechanisms of this gas, modes of antibiotic action as well as resistance while progressing towards new pharmacological targets to address drug resistance.



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G-Quadruplex Templated Synthesis of Selective Ligands

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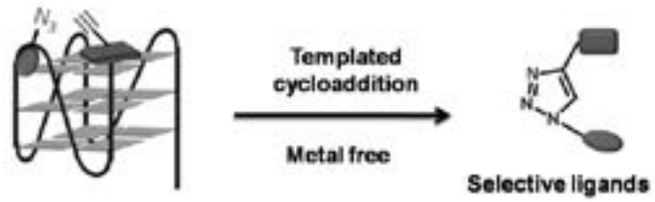
Small-molecules are fundamental probes for studying biological system. However, because of the dynamic nature of the biological macromolecules, the development of small-molecules that can interact with biological targets with high affinity and selectivity has always been challenging and time consuming. Target Guided Synthesis (TGS) shows a great promise in creating potent small-molecule probes for biomacromolecules by using them as the templates to assemble their own binders from a series of reactive molecular fragments. 1 I will present our recent work on innovative example of TGS by employing a G-quadruplexnano-template to catalyse the Huisgen cycloaddition between a variety of azide and alkyne fragments. The G-quadruplexnano-template has generated a triazolylcarbazole product,2-3 which is a selective fluorescent turn-on probe for the G-quadruplex over the duplex DNA. The carbazole ligand exhibits good cell penetration and anticancer properties. This work not only provides a novel strategy for controlled synthesis of G-quadruplex selective ligands but also offers an opportunity to recycle and reuse the DNA template.



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New Paradigms in the Synthesis of Privileged Heterocycles

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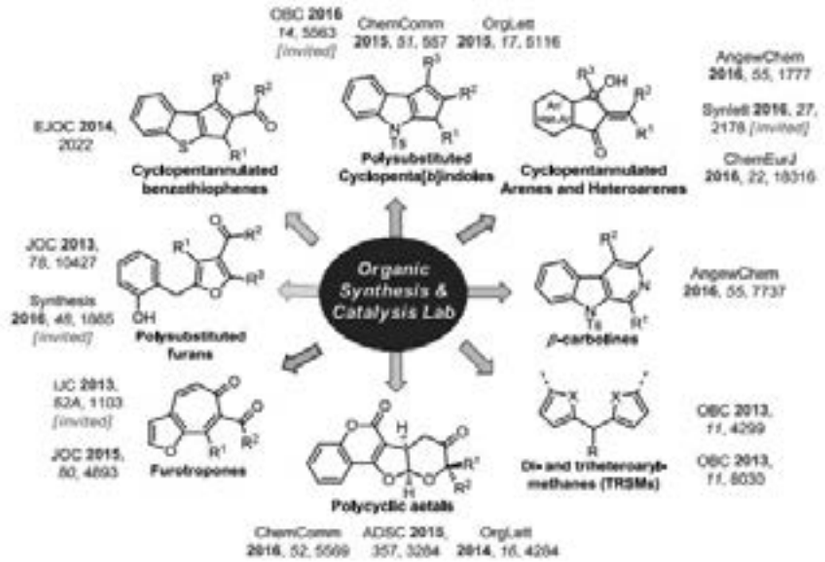
Heterocycles are common structural motifs present in over 80% of the currently marketed small-molecule drugs in market. Artificially mimicking the heteroatom containing biological molecules such as nucleic acids, amino acids, carbohydrates, vitamins and alkaloids in a subtle manner can lead to potential new drug candidates. Our lab has been actively involved in developing new synthetic strategies to access diverse classes of privileged heterocyclic scaffolds starting from readily available starting compounds. I am going to briefly talk about some of these efforts during my presentation.



Photoactive Metal-Based DNA Crosslinking Agents

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Two essential requirements of an anticancer drug are its specificity and efficacy. The platinum based cisplatin and its analogues as transcription inhibitors are well known for their chemotherapeutic activity. These nuclear DNA targeting drugs, however, suffer from undesirable side effects and procured resistance due to NER mechanism. One way to overcome such deficiencies is to develop anticancer agents showing activity via different reaction pathways, viz. intercalation to DNA, alkylation of DNA, topoisomerase activity, etc. Another viable way is to design DNA cross-linkers having appended photosensitizers such that a dual pathway can be operated with one part showing DNA transcription inhibition property while the photoactive moiety is suitable for to generation of reactive oxygen species (ROS) akin to the way known for photodynamic therapy (PDT). We have developed new ternary oxovanadium(IV) and platinum(II) complexes having photoactive moiety and labile ligands. Photo-activation of the complex results in damaging the cancer cells by producing ROS thus leaving any unexposed cells minimally affected. The ternary complexes that are susceptible to release ligand(s) generate two active species, one which can act as a transcription inhibitor, while other could show photo-induced cellular damage by generation of ROS. Specific delivery of the complex at various cellular organelles can be done by suitable designing of the complexes to achieve specificity and to augment the efficacy of the anticancer agents. Recent developments in this chemistry would be presented [1-3].

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Purpose Built Molecules for Theurapatic and Diagnostic Application

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Purpose-built molecules that are capable of functioning in predictive manner in presence of a certain external stimulation has significance for chemistry, clinical biology, diagnostic and photoactive smart material. Various photo-induced responses are being utilized for designing such photoactive molecules. Derivatives of ruthenium(II)-polypyridyl complexes/BODIPY or Rhodamine derivatives with varying photo-induced responses have been extensively used by researchers active in these areas. [1] Rich photophysical properties, stability of the photo-induced excited states and reversible redox behaviour are primarily accounted for this. Synthetic ease in achieving appropriate substitution of the coordinated 2,2'-bipyridy ligands (or its analog)/BODIPY or Rhodamine derivatives allows desired tuning of the energies of the frontier orbitals as well as the redox properties and the photoinduced excited states. These are crucial in designing complexes specific for each of these various applications. Our research interests include harnessing both coordinative interactions as well as various non-bonding interactions for realizing our goal. Noninvasive imaging approach is generally preferred for observing individual events in cells, as imaging studies are performed in physiologically authentic environments and have relevance for cell/molecular biology and studying bio-chemical processes. There are significant activities in designing appropriate imaging reagent for visualization of specific organelles with organelle-selective dyes in the membrane-enclosed intracellular structures, as this helps in gaining insight for monitoring important biological processes. [2,3,4] Stability towards photo-bleaching, cell membrane permeability, nominal cytotoxicity and luminescence in the longer wavelength following excitation with non-harmful visible light are some of the essential criteria for any such efficient imaging reagent. Keeping these crucial issues in mind, some of our recent efforts in the area of cellular imaging and photo-induced toxicity shall be discussed.

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POSTERS

P1

Genome Mining of A Hemibiotrophic Plant Pathogen Bipolaris Sorokinianaand Characterization of a Highly Stable Endoglucanase from the GH_7 Family

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Bipolaris sorokinianais a filamentous fungus that causes spot blotch disease in cereals like wheat, which have severe economic consequences. However information on the identities and role of the cell-wall-degrading enzymes (CWDE) in B. sorokiniana is limited. Many fungi produce CWDE like glycosyl hydrolase (GH) that help in host cell invasion. The first step towards understanding the role of these CWDE is to identify genes encoding such enzymes and characterizing them. We mined the genome of B.sorokinianato annotate homologs of five GH families: GH3, GH6, GH7, GH45 and GH61 (AA9) towards identifying the minimum set of GH families needed to hydrolyze biomass. Among them GH7 endoglucanases are one of the most important cellulolytic enzymes in nature towards industrial applications of cellulose breakdown. Bipolaris genome contains different number of paralogs for these five GH families and the relative transcript abundance of the paralogs were measured. The third homolog of GH7 (BsGH7-3) which shows higher level of transcript accumulation as compared to others was selected for further characterization. The recombinantly expressed GH7-3 enzyme is alkaliphilic with the pH optima being 8.1, thermostable having a temperature optima at 60 °C. The enzyme has a very long half life, with 65 % of residual activity after incubation for 365 hrs at 50 °C. The enzyme also shows stability towards salt, ionic liquid and most of the metal ions and thus positions itself in the robust group of enzymes that have many industrial applications.

P2

Understanding the Role of Non-Conserved Residues of β-Glucosidases in Increasing Glucose Tolerance

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The abundant plant biomass on earth has the potential to become a sustainable source of transport fuels. The economics of enzymatic hydrolysis of biomass into ethanol largely depends upon the performance of cellulase cocktail used for saccharification of the biomass. β-glucosidase (EC 3.2.1.21) is a vital component of cellulase and catalyses the hydrolysis of β-1,4 linkages of disaccharides or glucose substituted molecules into glucose. Most β-glucosidase (BG) is sensitive to their end product glucose, which is a limiting step in saccharification. Very little is known about the mechanism of glucose inhibition or the difference in glucose tolerance among BG's. Elucidation of the mechanism of glucose tolerance is thus crucial towards engineering high glucose tolerance and in turn efficient saccharification.

To understand the mechanism of glucose tolerance and identification of key residues responsible for glucose tolerance we have characterised two BG's, B8CYA8 from Halothermothrixorenii and O08324 from Thermococcus sp. Non-conserved residues based on multiple sequence alignment amongst BGs along and a rational design based strategy in the active site tunnel of the enzyme was used to design mutations. Biochemical characterisation of the mutants suggests that residues at entrance of the tunnel (gatekeeper) and inside the tunnel regulate the effect of glucose on catalysis. In this poster, we will present data that suggests that reducing steric hindrance at the entrance of the tunnel and the presence of hydrophobic residues in the active site tunnel of BGs leads to higher glucose tolerance. Our findings will be helpful in engineering active glucose sensitive BGs into glucose tolerant variants.

P3

Sterically Hindered Palladium(II) Complex: Anticancer Activity, Mechanism of Cell Killing and Docking Study

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In contrast to Pt complexes which are well known as anticancer agents most Pd complexes face a drawback of being very labile and not suitable for clinical use [1]. Steric hindrance is known to affect the rate of reaction due to the influence of the bulky electron envelope around the metal. Our approach is to use this concept for generation Pd complexes that would have potential in cancer chemotherapy. Mechanism of actions for these drugs involves activation after losing the labile ligand(s) in aqueous solution which is followed by binding with DNA. [2] They stop DNA replication and finally cell division although some resistance has been observed. But quick dissociation before reaching the target causes binding with deactivating biomolecules like glutathione in the cell. Our structurally characterized cis dichloro palladium(II) complexes bearing sterically hindered imidazole based Schiff base ligand is inspired by our reported observations on ruthenium(II) p-cymene complex. [3,4]. Complex (**1**) shows higher CT DNA binding constant in the order of 10^5 M^{-1} and is more stable to hydrolysis. At pH 6.7 hydrolysis rate increases significantly for both the complexes where as in presence of 110-130 mM chloride (extracellular chloride) the hydrolysis rate slightly decreases for **2**. Cellular toxicity studies show that **2** deactivates under hypoxic condition (IC_{50} = 31 μM (normoxia) and 43 μM (hypoxia) in MCF-7) but toxicity increases in presence of GSH (IC_{50} = 37 μM in MCF-7). However, GSH binding for both complexes is observed in UV-visible kinetics. Complex **2** arrests the cell cycle at G2/M Phase and follow apoptosis pathway of cell killing. Cell cycle accumulation study shows that complex **2** accumulates more than **1**.

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P4

Probing Supramolecular Structure and Orientation Using Fluorescence Mueller Matrix Spectroscopy

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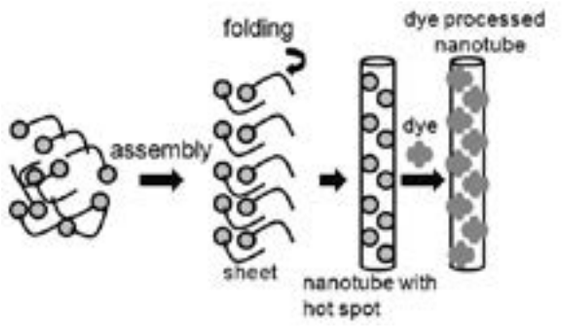
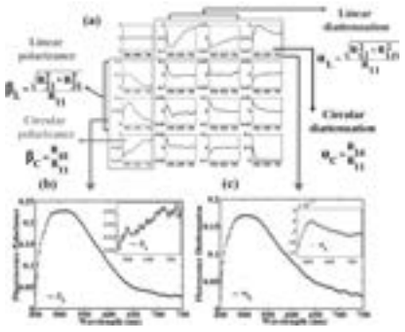
Self-assembly of peptide motifs to fabricate supramolecular nanotubesis a popular field of interdisciplinary research due to their wide applications in biology and material sciences. [1] Most of the reported motif contain either aromatic amino acids [2] or cyclic peptide for the fabrication of nanotube like structure. But the formation of the nanotube containg acyclic and non-aromatic are rarely explored. In this regards, fabrication of processable supramolecular nanotubes by molecular recognition, self-assembly and growth of a peptide motif Boc-Xaa-Met-OMe(Xaa = Val/ Leu) have been investigated. Probing the intermolecular interactions in supramolecular hybrid materials is highly important. The Met sulphurs are arranged helically along the supramolecular nanotubes like hot spot. The supramolecular nanotubes were processed with electron deficient dye TB-NDI. The formation of dye-supramolecular nanotubes hybrid has been proven by a novel method based on fluorescence spectroscopic Mueller matrix measurements and inverse analysis which effectively probe and quantify exclusive information on the molecular organization and orientation of dye around the supramolecular nanotubes via a set of newly defined fluorescence anisotropy parameters, namely, fluorescence diattenuation and polarizance. The report describes the fluorescence Mueller matrix probe on the helical arrangement of the achiral fluorescent dye molecules around the supramolecular nanotubes is promising for characterization of complex hybrid materials.





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P5

Exploring Novel Concepts in Spintronics with Exotic Molecules Made of Graphene Fragments

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Spintronics is an active area of research that explores novel physical phenomenon originating explicitly due to the spin degree of freedom of carrier electrons and aims to develop new type of devices by generating and manipulating spin polarized currents in non-magnetic conductors. Spin-dependent transport phenomenon arises primarily due to the presence of a significant spin-orbit coupling between the carriers and the medium. For example, when a charge current is induced in a conductor due to the application of an electric potential, a spin polarised current is generated in the transverse direction, a phenomenon known as Anomalous Hall Effect (AHE) in the case of ferromagnetic and Spin Hall Effect (SHE) for non-magnetic conductors. In contracts to AHE, SHE is not associated with any net electric potential which makes it extremely challenging to detect the phenomenon. Moreover, unlike charge current, spin current is a non-conserved quantity and decays drastically as it diffuses through a conductor. Thus a major challenge is to come up with new materials that will preserve spin current over significant length/time scales.

In the present work we showcase a new molecule denoted as Mn-Ply based on a ligand consisting of three fused benzene rings that can be viewed as a fragment of graphene. Ply has one unpaired electron delocalised over the entire planner ring and crystal packing arrangement of Mn-ply molecular solid shows that Ply ligand from two neighbouring molecules stack on top of one another with separation~3.7 Å. Thus, Mn-Ply is a promising material where injected spins can be envisaged to travel between molecules. With the goal of electrically detecting SHE, we have prepared devices consisting of trilayer structures of Cobalt/ Mn-Ply(5-20nm)/Copper, with the metallic electrode in cross stripe geometry. We perform low temperature electrical measurements in the so called 'non-local' mode, whereby current is passed through ferromagnetic electrode (Cobalt) only and voltage is measured in the non-magnetic electrode (copper). We argue that any measureable voltage in our measurement is due to the presence of spin current and present systematic data measured at low temperatures and applied magnetic field.

P6

Insight into the Dynamics of Zap70 in Activation and Downstream Signaling in T-Cells

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Protein tyrosine kinases are dynamic molecular switches that toggle between the inactive and the active state (1). The underlying mechanism of coupling between the signaling dynamics and the protein dynamics are poorly understood. We investigate how Zeta associated protein kinase (ZAP-70) dynamics regulates the activation of T-cell signaling. ZAP-70 (2) is comprised of tandem SH2 domain (t-SH2), which is made up of N-SH2 and C-SH2 domains, and a carboxy-terminal kinase domain. N-SH2 is connected to C-SH2 by interdomain A while interdomain B connects tSH2 domain with the kinase domain. Binding of antigen to T-cell receptor (TCR) results in phosphorylation of tyrosine of ITAM peptides in cytosolic domain of CD3-zeta (2). This leads to the recruitment of ZAP-70 to the membrane and thus activation of the protein. ZAP-70 binds to the ITAM of CD3-zeta at the membrane through t-SH2 domain (3). Structural analysis shows that TCR binding or phosphorylation of Zap70 triggers a transition from a closed autoinhibited conformation to an open conformation (4). Comparison of the secondary structure from NMR spectroscopic studies of ITAM-bound t-SH2 of ZAP-70 with crystal structure revealed three residues (hotspots)-F117, R121, W235 which are present especially in interdomain A. In the crystal structure, these residues, which are dynamic in nature, form a stacking interaction in the ITAM bound state. We hypothesize that this region might play an important role in the regulation of the protein dynamics and allosteric activation of ZAP-70. We will present the biochemical analysis to understand the function of stacking interaction in regulation of ZAP-70 activation in our poster.

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P7

Electronic Description on Photophysics of Homo and Hetero Dinuclear Cyclometalated Iridium and Rhodium Complexes

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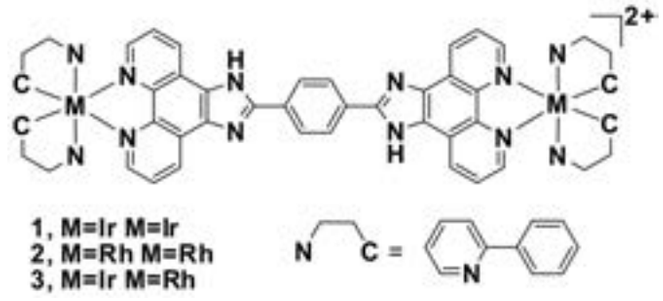
Photophysical properties of homodinuclear complexes 1 (Ir), 2 (Rh) and heterodinuclear complex 3 (Ir-Rh) have beendiscussed in solution and solid state with the help of quantum chemical calculations by combined DFT-TDDFT methods. Quantum calculations on these three complexes indicate participation of metal-to-ligand and ligand-to-ligand charge transfer to the lowest energy absorptions and electron transition from cyclometalating ligand to the ancillary ligand. The emission behaviour in the solution and solid state confirm the participation of triplet state as obtained from quantum chemical calculations. It is also noted that the emission behaviour in the mixed-metal complex is controlled by the iridium metal centre. The ground state electronic interaction between the metal centres studied by electrochemistry reveals weak interaction between them; however, energy transfer in the excited state is facile across the bridge.



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P8

Understanding the Role of Inositol Hexakisphosphatein the Activation of Bruton's Tyrosine Kinase

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Bruton's tyrosine kinase (Btk) is a non-receptor tyrosine kinase required for regulation of B-lymphocyte development, differentiation and signalling. Mutations in Btk lead to cancer, immunodeficiency diseases like X-linked agammaglobulinemia (XLA) for human and X-linked immunodeficiency (Xid) for mice. Btk is composed of an N-terminal Pleckstrin and Technology domain (PH-TH), Src homology 2 and 3 (SH2 and SH3) domains and the C-terminal tyrosine kinase domain. Btk is activated by its localization to the plasma membrane and subsequent phosphorylation by Src family of kinases (1). Recently, it was found that inositol hexakisphosphate (IP6) activates Btk,even in the absence of a membrane (2). IP6 binds to the PH-TH domain of Btk, which is hypothesized to stabilize a transient dimer of PH-TH domain. But, in spite of several evidences, the IP6 mediated dimer of Btk is yet to be detected in solution. In this study, we focus to characterize the IP6 mediated PH-TH dimer with the help of NMR spectroscopy. We also try to understand if IP6 plays any role in the constitutive activation of the E41K mutant of Btk.

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P9

Pyrazole Based β-Lactam Compound: Exploring Possible Role Against Dyslipidemiafrom Cholesterol Synthesis to Absorption

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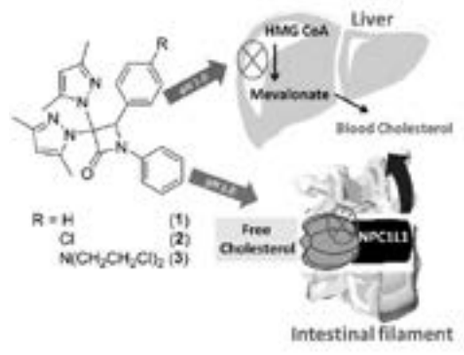
Cholesterol absorption and metabolism plays the critical role in dyslipidemia. To lower levels of bad cholesterol there are three major strategies (i) to target the mevalonate pathway (inhibit HMG-CoA reductase; clinical drug: statins) (ii) to decrease absorption of cholesterol from food (clinical drug: ezetimibe) (iii) reduced triglyceride synthesis and very low-density lipoprotein (VLDL) production (clinical drug: fibrates). There are strategies also to co administer statin to prevent choresterol synthesis 1 and ezetimibe (β-lactam based drug) for prevention of cholesterol absorption 2 in small intestine to reduce overall blood cholesterol levels. Inspired from such approaches we have developed bis-pyrazole based β-lactam compound with varying functionalities at the pyrazole based β- lactam core unit. All the analogues are stable enough to tackle extreme pHs inside our GI track. Our studies showed that one of the compounds bearing a mustard group shows toxicity against selected cancer cells where as the other analogues are not toxic within the experimental concentration (150 μM). Compound 1 and 2 are experimentally found to inhibit HMG-CoA reductatase, the key enzyme involved in esterification of cholesterol (IC50 for 2 is ~100 μM) but is inferior to statins. However, it also targets NPC1L1 as per our molecular docking studies. Results show that compounds 1 and 3 has higher affinity towards NPC1L1 even better than its known inhibitor ezetimibe from molecular docking scores.



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P10

Controlled Synthesis of Fluorescent Nanocluster by Templating Protein Fibrils

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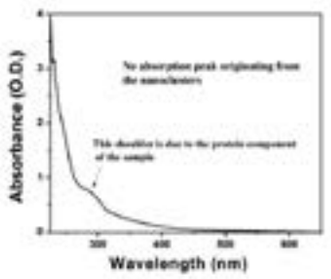
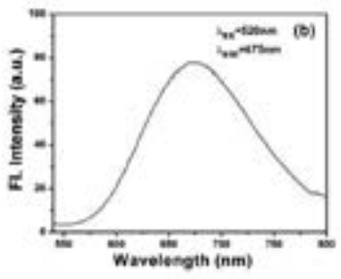
Fluorescent gold nanoclusters with sizes around 2 nm have been extensively investigated during the recent years for their promising applications in bio-imaging, sensing, single molecule optoelectronics, therapeutics and targeted delivery. 1, 2 Focus of interest ranges from fundamental properties such as photoluminescence, optical chirality, ferromagnetism, and redox like and quantized double layer charging behaviour. This is based on the particular size-dependent properties of the clusters. Many groups have been reported synthesis of various metal nanoclusters with magnificent optical properties using various biological scaffolds (e.g., proteins, DNA, peptide etc). 3 The use of biological templates have shown additional advantages of being nontoxic/biocompatible, greatly reduced size for enhanced cellular uptake, opportunity for two-photon absorption at biologically relevant wavelengths, etc.

In this study, we have synthesized fluorescent gold nanoclusters through the reduction of gold precursors (HAuCl¬4) by using bovine serum albumin in fibrillated form as template. The prepared nanoclusters have intense red emission with emission maxima (λem) at 675 nm upon being excited (λex) at 520 nm and therefore, assure formation of Au25 nanocluster. The as-prepared nanoclusters exhibit bi-exponential decay curve with a picoseconds lifetime.





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P11

Egg Shell Like Nanovesicles from Thiocoumarin Based ε-Amino Ester as Potential Carrier and pH Responsive Sustain Release

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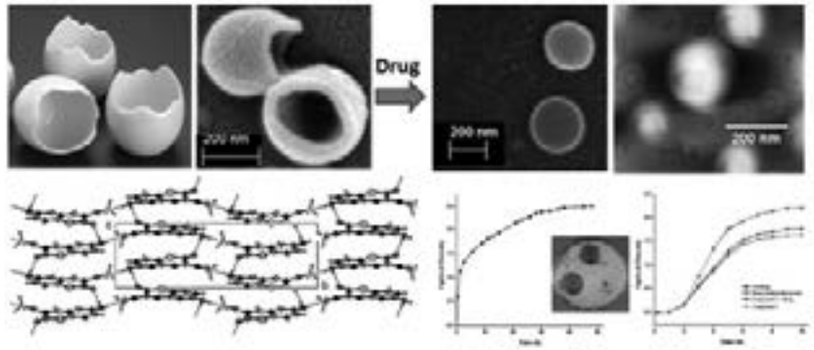
Naked drugs often cause systemic toxicity and unwanted side effects. [1] Hence pharmaceutical formulation is necessary. It is also important that the chemical substances should work in a synergy and will not do further reaction to avoid generation of harmful chemicals under physiological conditions. [2] In this regard self-assembled non coded amino acid based nanovesicles are promising [3] due to their biocompatibility, recognition properties, hydrophilic-hydrophobic balance and stability towards enzymatic degradation. [4] Here, we have synthesized and fully characterized the compound methyl 6-amino-2-oxo-2H-thio-chromene-3-carboxylate, a thiocoumarin based ε-amino ester from commercially available sources. [5] X-ray crystallography reveals that the ε-amino ester adopts porous architecture through multiple N-H….O and C-H….S intermolecular hydrogen bonding and π–π stacking interactions. The field emission scanning electron microscopy (FE-SEM) and the atomic force microscopy (AFM) revealed that the ε-amino ester exhibits egg shells like porous nanovesicles morphology. These egg shells like nanovesicles have been used as potential carrier for the bacteriostatic antibiotic sulfamethoxazole. The spectroscopic studies as well as the growth inhibition of E. Coli exhibit that the ε-amino ester-sulfamethoxazole formulation leads to pH responsive sustained release of the drug. The report highlights the utility of designer amino ester-drug supramolecular combination.



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P12

Inhibition of Insulin Amyloid Fibrillation by Heme and Its Derivatives

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Highly ordered structures from the self-assembly of proteins into amyloid fibrils is associated with various diseases in humans. Insulin is related to type-II diabetes and its amyloidosis was found at the site of insulin injection as well as in clinic formulation. We explored the effect of Heme and its derivatives; hematoporphyrin (HP), protoporphyrin IX (PP) on the in-vitro fibrillation of Insulin. The fibrillation kinetics was decreased on adding these compounds as evidenced by ThT fluorescence, characteristic of amyloid. This was further supported by scanning electron microscopy and circular dichroism where no insulin amyloid fibril has been detected. The conformational transition from α-helix to β-sheet probably arrested in the presence of these porphyrins, demonstrating that the native structures of insulin are protected in presence of these compounds. These results may provide a possible therapeutic strategy to prevent or treat insulin amyloidosis.

P13

Non Doped Electro Luminescent Device from C_3-Symetrical Organic Semiconductor: Improved E-& H^+ Mobility upon Thermal Annealing

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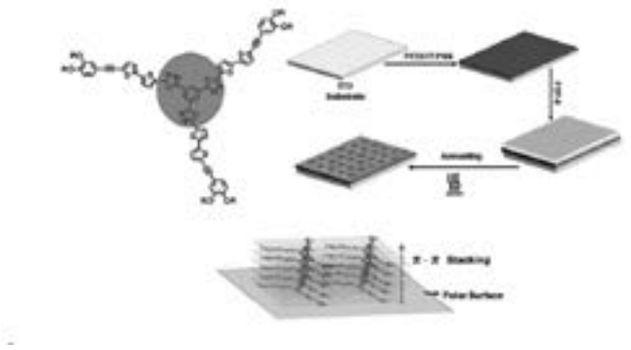
Balanced charge carrier mobility in organic semiconductor materials is important to accentuate them as superior active layer components in semiconductor devices such as ambipolar organic transistors (OFTs), organic photovoltaics (OPVs), and light-emitting diodes (OLEDs). Particularly for the development of flexible light emitting diodes, to simplify the layer structures if the emitting layer possesses balanced carrier mobility, bilayer device model may be adopted which will reduce the complexity of device structure. Here we describe interesting observation of balanced charge mobility upon thermal annealing in single carrier diodes of C3-symmetrical FDT-8 donor-acceptor molecule solely on polar underside layers. As the core unit of the molecule is symmetrically functionalized by 1, 3 oxadiazole unit which is well branded for its electron transport ability and at the same time towards the fringe by known hole transporting bis-thiophene unit, bipolar mobility is incorporated in to a single molecule. DFT molecular modelling concludes that the HOMO is centred to be at the core whereas the LUMO is localized at the periphery of molecule. These molecules is observed to have columnar stacking on thermal annealing on polar substrate and observed balanced carrier mobility in their single carrier diodes. Bilayer electroluminescent devices fabricated out from FDT-8 possess a turn on voltage of 4 V and a maximum current efficiency of 2.4 cd/A obtained for the best device.



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P14

Fe(IV)–Oxo–Hydroxo Oxidant Mediated Intramolecular Ligand Hydroxylation and Role of Lewis acid on O-O Bond Cleavage: A DFT Study

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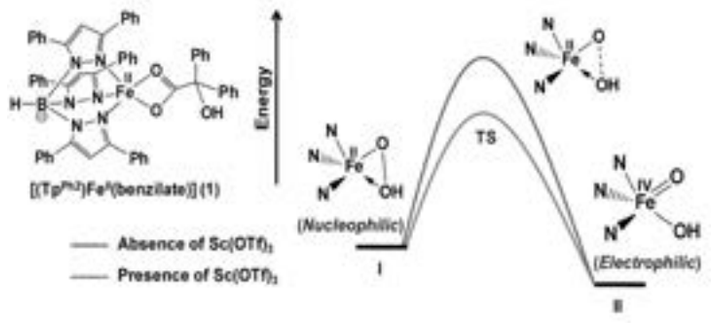
Over the last decades, biomimetic oxidation of alkanes and alkenes by iron complexes in the presence of “ready oxidant” H2O2 has been extensively studied. Several iron–oxygen intermediates such as iron(III)–(hydro)peroxo and iron(IV)–oxo species have been generated through reduction of dioxygen by iron(II) complexes. However, the selective oxidation of C–H and C=C bonds by biomimetic complexes using O2 are rare and remains a major challenge in bioinspired catalysis. In this endeavour, a nucleophilic side-on FeII–hydroperoxo oxidant (I) is proposed to form in the reaction of high-spin iron(II) complex [(TpPh2)FeII(benzilate)] (1) [TpPh2=hydrotris(3,5-diphenylpyrazolyl)borate] with dioxygen in benzene at ambient temperature. [1] The concomitant decarboxylation of benzilic acid yields benzophenone. I undergoes O–O bond cleavage to generate an electrophilic FeIV–oxo–hydroxo oxidant (II). The dissociation of O–O bond is facilitated in the presence of a Lewis acid e.g.Sc(OTf)3. [2] The novel oxidant II exhibits versatile reactivity e.g.cis-dihydroxylation of alkenes, selective oxidization of sulfides to sulfoxides and hydroxylation the strong aliphatic C–H bonds. In the absence of any substrate, the oxidant intramolecularly hydroxylates one of the phenyl rings at ortho position on the facial tridentate TpPh2 ligand. We have performed DFT calculations to investigate the energetics of the O–O bond cleavage of FeII–hydroperoxo species prior to the generation of active electrophilic oxidant both in the absence and presence of Sc(OTf)3. Emphasis is also placed on the detailed mechanism of the intramolecular ligand hydroxylation and activation of strong C–H bond of cyclohexane by the electrophilic oxidant followed by the stereoselective hydroxylation.



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P15

Holographic superconductors

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Based on the Sturm-Liouville eigenvalue problem, we analytically investigate several properties of holographic s-wave superconductors in the background of a Schwarzschild-AdSspacetime in the framework of Born-Infeld electrodynamics. Based on a perturbative approach, we explicitly find the relation between the critical temperature and the charge density and also the fact that the Born-Infeld coupling parameter indeed affects the formation of scalar hair at low temperatures. Higher value of the Born-Infeld parameter results in a harder condensation to form. We further compute the critical exponent associated with the condensation near the critical temperature. The analytical results obtained are found to be in good agreement with the existing numerical results.

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P16

C–F Bond Activation by Group 14Dialkylamino Metalylenes: A Competition Between Oxidative Addition vs. Substitution Reactions

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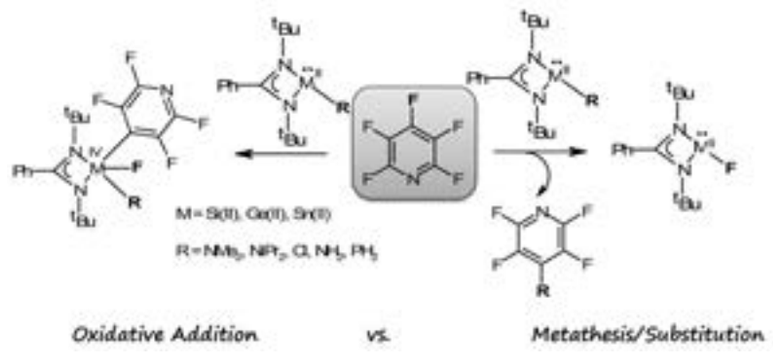
The importance of the C–F bond continues to draw attention of the scientific community owing to their necessity in both industrial and academic research. [1] The high electronegativity and small size of the fluorine atom makes C–F bond strongest among all the single bonds that carbon forms with any atom. Because of these particular features, C–F bonds show exceptional kinetic inertness and it becomes highly challenging to activate the bond in mild reaction conditions. Recently, Roesky et al. have reported the activation of C–F bond of pentafluropyridine by Group14 dialkylaminometalylenes. [2] They have found two different mode of reactivity depending on the M(II) atom [M=Si, Ge, Sn] and basicity of the substituent present at the M(II) (Scheme 1). Emphasis is placed on the underlying mechanistic principle using state-of-the-art theoretical methods to provide a systematic classification of the individual mode of reactions. In an attempt to clarify the mechanistic issues, few pertinent questions are of high relevance in this current context: i) What is the role of different metal for switching the selectivity? ii) What is the role of different substituents on reactivity and selectivity? iii) Why preferably para C–F bond is activated? Finally, an Energy Decomposition Analysis (EDA) is invoked to get brief insight into the physical factors that control the activation barriers originating via different reaction modes, viz. oxidative addition and substitution/metathesis. We hope the results will provide ample guidance to the experimentalists to design better reaction conditions.



Scheme 1. Different mode of reactivity of Group 14 DialkylaminoMetalylenes

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P17

Dual Fluorescence of Green Fluorescent Protein (GFP) Chromophore Analogues and its Chemical Modulation

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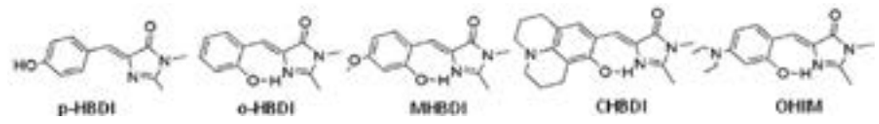
Green Fluorescent Protein (GFP) has been extensively used in bioimaging.1 In order to understand fluorescence behaviour of GFP researchers have chemically modulated GFP chromophore (p-HBDI) and have observed either charge transfer (CT) or proton transfer (PT) band an analogues of GFP chromophores. 2 Dual fluorescence has been an interesting topic to spectroscopists. 3 However, there is no such report of dual fluorescence in GFP chromophore analogues.

In order to observe dual fluorescence three structurally different GFP chromophore analogues (OHIM, CHBDI, MHBDI) have been synthesized (see chart below). The ability of charge transfer donation as well as structural restriction are different in these three molecules. Out of these three molecules OHIM exhibits only CT band, CHBDI exhibits dual fluorescence-equal intensity both CT and PT bands, whereas MHBDI exhibits dual fluorescence-higher intensity PT band in comparison to CT band. The relative ratio of CT and PT bands could be modulated by polarity of the solvents. When embedded in polymer matrix optical behaviour of these molecules changes significantly. For example fluorescence quantum yield as well as fluorescence lifetime gets enhanced by more than an order of two. These optical behaviour could be explained by electronic energy level diagrams. All these results will be elaborated.



Scheme 1. Different mode of reactivity of Group 14 DialkylaminoMetalylenes

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P18

Spectroscopic, Structural and Computational Studies of Dirhenium Complexes Incorporating the Guanidinato and Dithiocarbamato Ligands

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The biological and therapeutic properties of some guanidine and dithiocarbamate compounds have fuelled the interest in developing the chemistry of those two ligands. Only a few guanidinate and dithiocarbamate complexes of dirhenium have been reported [1]. In pursuit of our general interest on the chemistry of dirhenium, we have been investigating the fundamental chemistry of dirhenium incorporating different guanidinate and dithiocarbamate ligands. The reason for this investigation is that the guanidinate and dithiocarbamate ligands have not been extensively applied to the dirhenium chemistry. In the course of this investigation we have discovered that triphenylguanidine (HTPG) reacts with $[Re_2(\mu\text{-}O_2CCH_3)_4Cl_2]$ to give the mixed μ- acetate/μ- guanidinate complex, $[Re_2(TPG)_3(\mu\text{-}O_2CCH_3)Cl]Cl$ as well as the mononuclear Re(VII) compound $[H_2TPG][ReO_4]$, the product being determined by the choice of reaction solvent[2]. Whereas HTPG promoted ortho-metalation reaction has been observed in the reaction between the $Re_2Cl_4(\mu\text{-}Ph_2PCH_2PPh_2)_2$ and different para-substituted triphenyl guanidine ligands (HTPGR, R = H, Me, OMe) in refluxing ethanol [3]. This is the first example of ortho-metalateddirhenium complexes with the bridging dppm ligands. On the other hand different dithiocarbamate ligands react with $Re_2(\mu\text{-}O_2CCH_3)Cl_4(\mu\text{-}Ph_2PCH_2PPh_2)_2$ in refluxing ethanol to afford the paramagnetic substitution products[4] of the type $Re_2(\eta^2\text{-}S,S)_2(\mu\text{-}S,S)(\mu\text{-}Cl)_2(\mu\text{-}Ph_2PCH_2PPh_2)$ where S,S = S_2CNMe_2, S_2CNEt_2, and $S_2CN(CH_2)_4$. These are the first example of dirhenium complexes that contain bridging dithiocarbamato ligand along with the dppm ligand. Aiming at the extension of these studies and further exploration of the reactivity of dirhenium towards different dithiocarbamate ligands, different dirhenium synthons were reacted with various dithiocarbamate ligands. The syntheses, structures and properties along with the theoretical studies of the new dirhenium complexes derived from the reactions of different dirhenium synthons with various dithiocarbamate ligands will be presented.

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P19

Calcium Phosphate Quercetin Nanocomposite And Its Applications

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Calcium phosphate quercetin nanocomposite (CPQN) i.e., quercetin entrapped in calcium phosphate nanoparticle was synthesized by a precipitation method at 800C, using di-ammonium hydrogen phosphate, calcium nitrate and quercetin as precursors and sodium citrate as stabilizer. The nanocomposite suspension had different color, size, shape, and stability at different pH. In addition, the CPQN had high fluorescence property with two emission peaks at 460 and 497 nm, when excited at 370 nm. Therefore, by the color changing property, CPQN may be used as a pH indicator and by its high fluorescence property, it may be used as effective fluorophore to label biological cell. Moreover, the nanocomposite had potential anti-oxidant property, for which CPQN was found to neutralize the deleterious effects of H2O2 viz., cell death, generation of intracellular reactive oxygen species and loss of connectivity in mouse neural cells. Therefore, CPQN might have potential use in future as an anti-oxidant drug.

P20

Coordination chemistry of platinum: Chelation isomerism and targeted metallation

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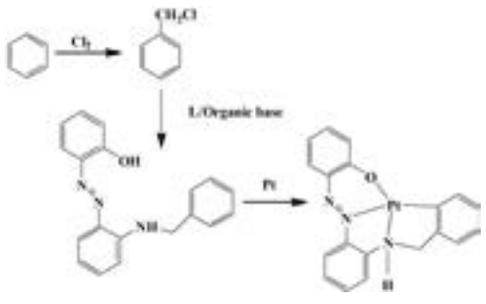
Coordination chemistry of platinum metals has been developed considerably during the last few decades due to their potential applications in catalysis, chemotherapy and their ability to exhibit versatile interesting physical properties. As a result new chelating ligands are being designed and synthesized to explore the chemistry of platinum by the researchers. The diversity in chelation property is one of the important objectives to employ the azo ligands to study the coordination chemistry of transition metal ions. Two types of expected chelation modes of azo ligands prepared by us are given below. In reality, only Pt(II) formed both type of chelates which may be termed as chelation isomers.

However, such diversity in chelation modes provided the opportunity to search the possibility of targeted metallation. Thus we wanted to find the way of carrying out regiospecific metallation at a specific ortho carbon of toluene according to the scheme given below. The strategy may be considered as the precondition for activation of specific ortho carbon of toluene for appropriate functionalization.



P21

Formation and Stabilization of μ_5-PO_4-Bridged Decanuclear Metallomacrocyclic [Zn^{II}_{10}] and μ_4-$HAsO_4$-Bridged Tetranuclear [Zn^{II}_4] Clusters

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Reaction of a newly synthesized five-coordinate dinuclear zinc complex, $[Zn_2(cpdp)(H_2O)_2]Cl$ (1) (H_3cpdp = N,N'-Bis[2-carboxybenzomethyl]-N,N'-Bis[2-pyridylmethyl]-1,3-diaminopropan-2-ol) with $Na_2HPO_4{\cdot}2H_2O$ in methanol-water at ambient temperature produced a novel phosphate-bridged decanuclear zinc cluster, $(H_3O)_4[Zn_{10}(cpdp)_4(\mu_5\text{-}PO_4)_2(H_2O)_6](6Cl){\cdot}53H_2O$ (2). In contrast, reaction of 1 with $Na_2HAsO_4{\cdot}7H_2O$ in methanol-water in the presence of NaBr at ambient temperature yielded a novel hydrogen arsenate-bridged tetranuclear zinc cluster, $Na_2[Zn_4(cpdp)_2(\mu_4\text{-}HAsO_4)]ClBr{\cdot}13H_2O$ (3). Single crystal X-ray structure analysis reveals that cluster 2 shows a $\mu_5{:}\eta^2{:}\eta^1{:}\eta^1{:}\eta^1$bridging mode of two PO_4^{3-} groups with each bridging among five zinc(II) ions. Cluster 2 is an interesting example of a μ_5-PO_4decanuclearzinc cluster forming a 16-membered $Zn_4O_8C_2P_2$metallomacrocyclic ring. Cluster 3 displays a $\mu_4{:}\eta^1{:}\eta^1{:}\eta^1{:}\eta^1$bridging mode of the $HAsO_4^{2-}$ group connecting four zinc(II) ions as revealed by its single crystal X-ray structure analysis. In solution, the UV-Vis titration spectra show the binding-induced significant increase in the absorption intensities of complex 1, accompanied by a substantial red shift upon increasing the concentration of PO_4^{3-} and $HAsO_4^{2-}$ anions. In addition, the integrity of 1, 2 and 3 in solution, has been confirmed by ^{1}H and ^{13}C NMR spectroscopy. Thermal properties of 2 and 3have been investigated by thermogravimetric analyses.

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P22

Bio-Inspired Mononuclear Copper(II) Complex with Labile Coordination Site: Galactose Oxidase Modeling and Alkane Oxidation

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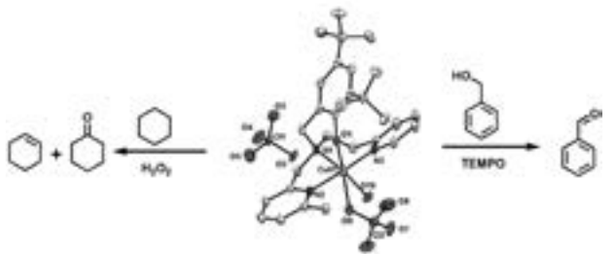
The modeling of the galactose oxidase has drawn an appreciable attention to the chemists' mind, especially after the X-ray structure determination of the protein active site.1 Galactose Oxidase (GOase) is a mononuclear copper oxidase. It uses a modified tyrosyl radical to ease the two- electron oxidation of primary alcohol to aldehyde with subsequent reduction of dioxygen to peroxide. 2 Oxidation chemistry of the metal complexes has now been extensively developed, affording the detail study of the mechanistic pathways of useful homogeneous catalytic reactions and radical-based enzymatic reactions. Among them the catalytic oxidation of alcohol is an important transformation from the perspective of organic synthesis as well as industrial purpose. 3 In this context, the present work is purposefully manifested to elucidate the structural feature essential for GOase reactivity through functional model chemistry on the basis of its' economic and environmental viewpoints. Here it fulfills the urgent demand of greener and more atom-efficient methods that employ clean oxidants such as O2 and H2O2 and a (preferably recyclable) catalyst. This GOase model complex reproduces many unique properties of the GOase including its catalytic conversion of primary alcohol to an aldehyde as well as cyclohexane to cyclohexanone in the presence of TEMPO (2,2,6,6-Tetramethylpiperidine-1-oxyl) and H2O2.



Synthetic Scheme of oxidation reaction by Galactose Oxidase model Complex [CuII(HLMe)(H2O) ClO4]ClO4

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P23

Exploration of Soft Oxometalates in Patterning and Allied Studies

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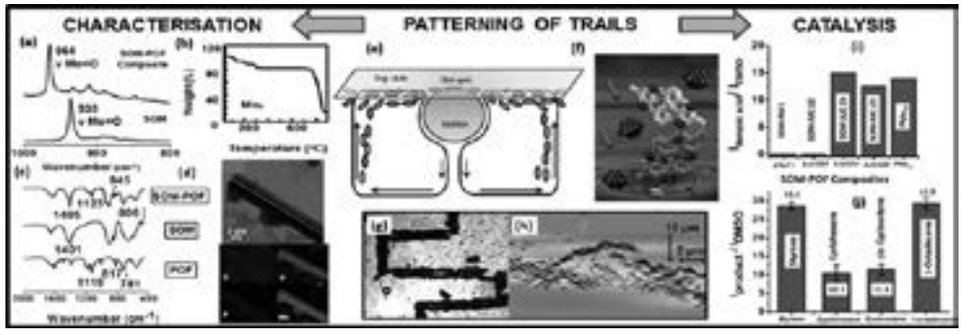
Soft oxometalates or SOMs are the heterogeneous dispersions formed by polyoxometalates of colloidal length in solutions. [1] These are intermediate of molecular POM solutions and their crystalline counterparts. [1] In this presentation, we shall depict controlled nucleation of SOMs to form microdimensional arrays of POMs using laser irradiation of thermo-optical tweezers. [2] The patterning process involves a phase transition phenomenon where SOM colloids are transitioning to polycrystalline POM arrays (Figure 1 g. and 1 h.) .[2] Further, these arrays have demonstrated their function as 2D catalytic chemical reactionwares, for instance, SOMs along with various POFs (Porous organic frameworks) have been shown to form inorganic-organic hybrids which on patterning act as robust catalysts (Figure 1 a- d) for oxidation of aliphatic and aromatic aldehydes (Figure 1 i). [3] Additionally trails formed from SOMs have exhibited catalysis of epoxidation of alkenes in a site specific fashion (Figure 1j). [4]



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P24

Zn^{II}–MEDIATED LIGAND RADICAL-DRIVEN -O-CH_2-O- BOND FORMATION

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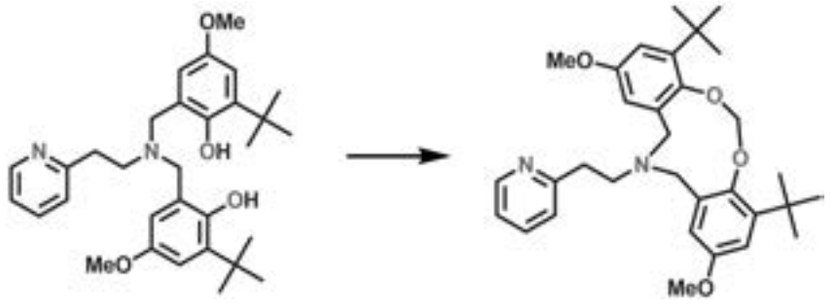
The interplay of transition metal ions and redox-active proradical ligands and the correlation of reactivity with electronic structure is an area of significant current research interest. Because of redox-active character these ligands have the ability to span oxidation levels to store redox equivalents. 1 Due to the lower redox potential of redox-active moieties, these often have enabled catalysis and multi-electron stoichiometric reactions, especially the processing of small molecules is prevalent in enzymology.[2]In this presentation, a new tripodal N_2O_2-donor ligand having pyridine and substituted redox-active phenolic moieties, has been synthesized. Upon stoichiometric reactions of Zn^{II}-salts in the presence of Et_3N, under aerobic condition affords radical-driven an unprecedented cyclic acetal formation through dichloromethane activation (used as a solvent with methanol), 3 whereas a tetra-coordinated ZnII complex was obtained in chloroform/carbon tetrachloride (used as a solvent with methanol). This unusual cyclised acetal formation thoroughly characterized both structurally and electronically.



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P25

Alanine Containing Cationic Polymer Induced Actin Polymerization

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Actin is a ubiquitous protein found in many living organisms and cells such as cell migration, cell division, wound healing, synaptic plasticity, immune response and host response to pathogens. The polymerization of actin, in vivo and in vitro, is induced by the presence several natural and synthetic compounds which are able to bind actin and alter the actin filaments dynamics via nonspecific electrostatic interaction between negatively charged actin and positively charged compound [1]. With the aim of developing a new cationic polymer, we have first synthesized poly (tert-butyl carbamate (Boc)-L-alanine methacryloyloxyethyl ester) (P(Boc-Ala-HEMA)) homopolymer in a controlled fashion by the reversible addition-fragmentation chain transfer (RAFT) polymerization. Subsequent deprotection of Boc groups in the homopolymer under acidic conditions resulted positively charged polymer with primary amine moieties at the side chains. This cationic polymer (P(NH_3^+-Ala-HEMA)), is able to transform monomeric G-actin to filamentous F-actin *in vitro* (Figure 1). These polymers are nontoxic to the cultured HeLa cells and also stabilize the filamentous actin inside the cells [2].

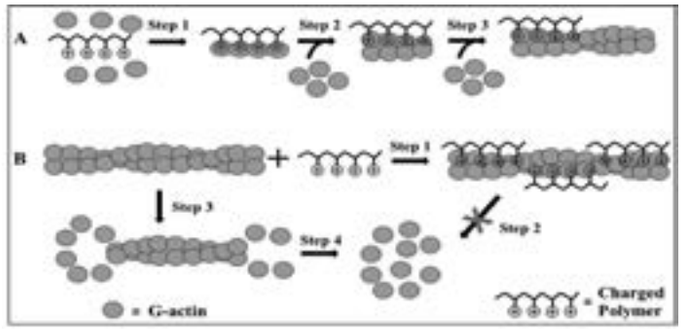

Figure 1. Mechanism of actin polymerization and depolymerization.

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P26

Polymer-Chlorambucil Drug Conjugates: A Dynamic Platform of Anticancer Drug Delivery

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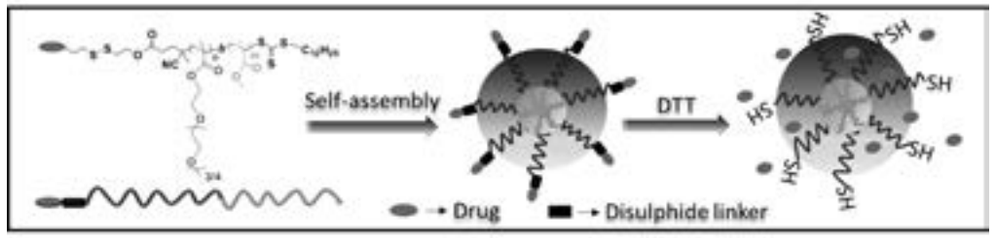
therapy. Among many types of alkylating agents, the nitrogen mustard chlorambucil (CBL) is one of the classic examples of bifunctional alkylating agent as anticancer drug, which has already been approved for cancer treatment. The nitrogen mustard moiety in CBL is the most attractive part, because it interferes in the replication of deoxyribonucleic acid (DNA) through the alkylation of nucleobases by forming aziridinium ion as an intermediate and it is important to mention that carboxylic side in CBL is pharmacokinetic but not dynamic. Therefore, binding of a non-toxic molecule to this carboxylic side of CBL will only affect its absorption and half-life, not the effectiveness. At present, the polymeric prodrugs have attracted considerable attention to achieve low toxicity and potential drug delivery towards cancer cells. Polymer-drug conjugates (PDCs) in which drug molecules are covalently bound to polymeric systems via biodegradable linkers are promising co-delivery carriers. In this work, we have developed a simple strategy to make PDCs of an antitumor alkylating agent, chlorambucil, using a biocompatible disulphide linker. Chlorambucil based chain transfer agent was used to prepare various homopolymers and block copolymers in a controlled fashion via reversible addition-fragmentation chain transfer (RAFT) polymerization. Chlorambucil conjugated block copolymer, poly (polyethylene glycol monomethyl ether methacrylate)-b-poly(methyl methacrylate) (PPEGMA-b-PMMA) formed well-defined spherical nanoparticles (NPs) in aqueous medium, as confirmed by 1H NMR, DLS and FE-SEM study. The block copolymer enabled the release of CBL in the presence of D, L-dithiothreitol (DTT) as reducing agent and also can load hydrophobic dye/drug molecules. In response to reductive reactions, CBL released from the micelles does not affect the aggregated nature of PPEGMA-b-PMMA, which was confirmed by DLS and FE-SEM study. These significant results suggest that a well-defined thiol-responsive spherical NP can act as a drug-delivery systems (DDS) towards cancer therapy through alkylating the nucleobases of DNA.



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P27

A Copper-Based Catalyst for Poly-Urethane Synthesis from Discarded Motherboard

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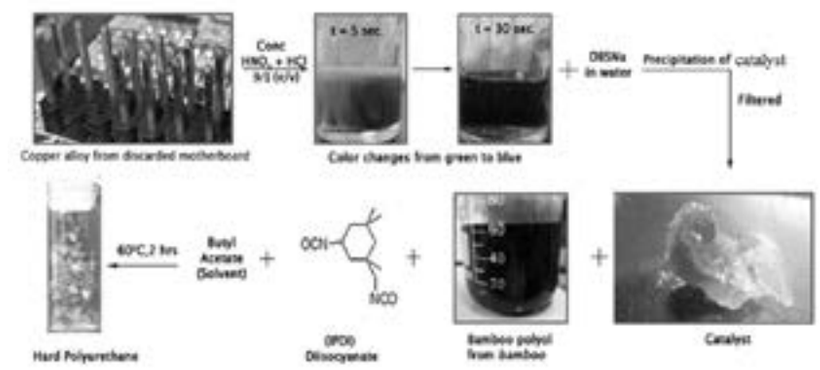
By displaying thermoplastic, elastomeric and thermoset behavior depending on their chemical and morphological properties, polyurethanes have caught attention since 1937 when Bayer and his co-workers made them for the first time using the reaction of polyester diol and isocyanate.[1] To produce a great range of versatility, various isocyanates can be used for making linear or cross-linked polyurethanes.[2,3] Here we used IPDI as isocyanate and bamboo polyol as polyalcohol to prepare hard polyurethane and polyurethane foam. A cheap copper-based catalyst has been synthesized from discarded motherboard to replace the industrially used tin-based catalyst.[4]



DBTDL [dibutyltin(IV) dilaurate] which is expensive and we found almost similar productivity compared to conventional catalyst DBTDL. By optimizing catalyst loading, time and temperature, a 97% yield was obtained with 1.8 mol% catalyst loading in 2 hours. A plausible mechanism has also been proposed.

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P28

Multi-functionalized Microporous Polymeric Network: An Efficient Tool for Removal of Toxicants

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Unlike non-degradable metal based adsorbents such as Zeolite and Metal Organic Framework (MOF), biodegradable Polymeric Organic Framework (POF) can prove to be a vital tool for adsorption of toxicants. Controlled architectural designed networks with and without functionalization can show specific selectivity towards toxicants. Rigidity and insolubility in aqueous phase are the desired property towards its development. We have successfully prepared covalently crosslinked POF network with high strain, high stain and high swelling capacity that too via facile synthetic route. Certain dyes and toxic heavy metals such as mercury (Hg), arsenic (As), cadmium (Cd), etc are Low Molecular Weight (LMW) toxicants. They interfere with the body metabolism. Therefore, their removal is most essential. We have successfully demonstrated that using our newly developed functionalized POF's, the organic dyes and non-degradable inorganic toxicants are trapped significantly.

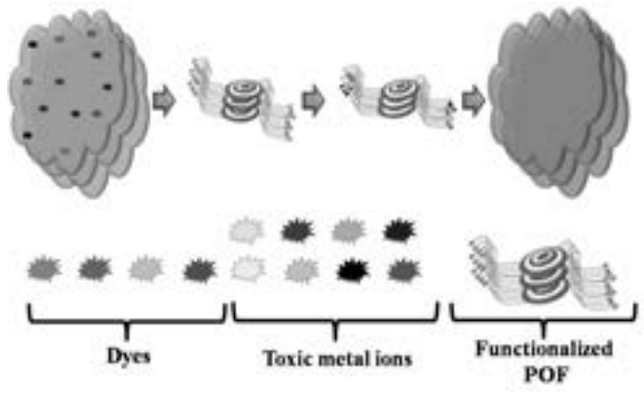

Figure 1. Pictorial representation of purification of aqueous system via removal of toxicant using functionalized POF as trapper.

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P29

Norbornene Based Copolymer for Site-specific Theranostic Application

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Theranostic is a concept, deals with therapy and diagnosis which actually helps to increase the survival rate against the terminal illness. Cancer is one of those which cause a huge death in each year, so early detection of cancer helps to start the proper treatment which increases the survival rates. Polymeric systems are having widespread application in biomedical field due to their high biodistribution and retention effect. Among several polymerization techniques Ring opening metathesis polymerization (ROMP) is a versatile technique to make highly functional polymers for biomedical application due to its functional group tolerance. So different norbornene based copolymers have been synthesized for the purpose of diagnosis and therapy simultaneously. The presence of imaging agent also helps to monitor the therapeutic pathway. Inclusion of site-specific group to the polymeric backbone reduces the cytotoxicity towards the normal cells.

Figure 2. Cartoon demonstration of nano-theranostic agent

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P30

Ligand sensitized strong luminescence from Eu^{3+}-doped $LiYF_4$ nanocrystals: A photon downshifting strategy to improve the Si solar cell efficiency

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Luminescence from Ln3+-doped nanomaterials are useful for various applications such as developing economical luminescent lamps, light emitting diodes, television and computer displays, optical fibres, lasers, just to mention a few. The interest in Ln3+-doped materials stems from their sharp f→*f*transitions which are forbidden by the Laporte selection rule. This leads to low absorption and consequently low luminescence quantum yield (QY).This demands for methods to improve their QY via sensitization. Generally, this is achieved using organic molecules but the method is restricted to lanthanide complexes. We have for the first time developed a simple ligand exchange approach to attach 4,4,4-trifluoro-1-phenyl-1,3 butanedione (TPB) to the surface of Eu3+-doped LiYF4 nanocrystals (NCs). The reason for choosing TPB ligands is due to their broad UV absorbance which has a strong overlap with the excited Eu3+ energy levels. Upon excitation of the ligand in UV region, very efficient energy transfer take places from the ligand to Eu3+ ions, leading to a very intense red emission. The sensitization of Eu3+ ions enhances the quantum yields (~31 %) of Eu3+ ions compared to ~5% via direct excitation of Eu3+ ions (Ex 394 nm) in Eu3+-doped LiYF4 NCs. The broadband ultraviolet excitation and intense red emission of Eu3+ ions have been explored for the enhancement of solar cell efficiency.1 This is done by depositing the nanocrystals on the surface of quartz and then that quartz was kept on the top of silicon solar cell.

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