Memorial Lectures

Prof.M.K.Rout Memorial lecture

Diverse Organic Synthesis, Functional Materials for Nanoelectronics, Sensors and Smart Devices

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Abstract: My research group is dedicated for diverse synthesis of organic compounds through C-H Activation, Photocatalysis, NHC-Catalysis, Organocatalysis and Dual Catalysis.[1]The organic electronic products are also lighter, more flexible, biodegradable, inexpensive, and ease to purify, fabricating devices and modify electronic environment. Thus, semiconducting, electronic and optoelectronic properties can easily be modified through changing size, shape, chemical structure, morphology and installation of a wide range of functional groups, which in turn generates innovative semiconducting, conducting, photoluminescence, storage, display and chemosensing performances to achieve highly efficient new generation electronic devices.[2] Thus, design and synthesis of new organic compounds as varied probes, their fabricated unidirectional materials and development of especially new chemo sensing property are desirable for achieving sensor devices of ultimate sensitivity.We have developed several organic probes and materials for sensing poisonous gases. phosphates, hydrazines, cyanide, heavy metal ions and other analytes.[3] For instance,fabrication of organic nanofibrils using 3-oxime-4-hydroxy-1,8-naphthalic-nbutylimide (**R1**)-doped polycaprolactone (PCL) electrospun used as a gaseous phosgene-specific sensing device. Herein, the higher surface to volume ratio and innovative properties of the nanofiber mats exhibits diminution of response time in comparison to the composite film of the same materials. Proficient gas penetration confers a fast chemical reaction, which is linear to the phosgene concentration and delivers a very low detection limit of 0.087 ppm. Importantly, LOD of gaseous phosgene in all type of solid-protocols used is far lower than the safety level phosgene concentration to human exposure.[3g]Our designed organic and polymer nanomaterials also capture heavy metals and gases and making our mother nature clean, safe and harmless.[4]

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Prof.S.R.Mohanty Lecture

BREAKING BONDS TO ORDER – A DREAM STILL ALIVE?

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Abstract: Skilled blending of the accumulated wisdom about electronic and vibrational excited states with new tools such as Lasers and High Energy Accelerators has opened new avenues of using photons as versatile chemical reagents to crack molecules to order and produce new Chemistry. The advent of high power infrared laser has given birth to a new Chemistry "Vibrational Photochemistry". This selective Photochemistry has opened up new possibilities of probing molecular dissociation, isomerisation and finally raised hopes (!) of bond selective Chemistry.

Excitement and fun of participation in this Laser Alchemy (?) will be shared.

Periodic Table Presentations

Periodic Table Presentation:01

Evolution of Periodic Table

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Abstract: This year we are celebrating 150th year of periodic table of elements on the eve of declaration of the first periodic table by Dmitri Mendeleev in 1869.

First systemization attempts of the then known 33 chemical elements were made in 1789 by Antoine Lavoisier who grouped them into gases, metals, nonmetals and earths. In 1829, Johann Wolfgang Döbereiner observed that many of the elements could be grouped into triads based on their chemical properties. Döbereiner also observed that, when arranged by atomic weight, the second member of each triad was roughly the average of the first and the third.In 1862, the French geologist Alexandre-Émile Béguyer de Chancourtois published an early form of the periodic table. He called it telluric helix or screw. He was the first person to notice the periodicity of the elements. With the elements arranged in a spiral on a cylinder by order of increasing atomic weight, de Chancourtois showed that elements with similar properties seemed to occur at regular intervals.

In 1864, Julius Lothar Meyer, a German chemist, published a table with 28 elements. A missing element between Si and Sn was predicted with atomic weight 73 and valency 4.In 1866, English chemist John Newlands when listed the elements in order of increasing atomic weight, similar physical and chemical properties recurred at intervals of eight. He likened such periodicity to the octaves of music.

Dmitri Ivanovich Mendeleev,a Russian chemist, formulated the Periodic Law. He is often referred to as the Father of the Periodic Table. He called his table or matrix, "the Periodic System". On 6 March 1869, he made a formal presentation to the Russian Chemical Society, titled *The Dependence between the Properties of the Atomic Weights of the Elements*, which described elements according to both atomic weight and valence. Mendeleev has the distinction of accurately predicting the qualities of what he called ekasilicon, ekaaluminium and ekaboron (germanium, gallium and scandium, respectively).

In 1911, Dutch Physicist Antonius van den Broek was the first to propose that “Atomic number (nuclear charge) determined the placement of elements in the periodic table”. Henry Moseley tested Broek’s hypothesis by investigating the Fraunhofer lines of various elements. He found a relationship between the X-ray wavelength of element and its atomic number.Later advances like discovery of electron and radioactivity by the end of 19th century revolutionized the modern structure of the elements and long form.

An extended periodic table theorizes about chemical elements beyond atomic number 118.If further elements with higher atomic numbers than this are discovered, they will be placed in additional periods. Any additional periods are expected to contain a larger number of elements than the seventh period, as they are calculated to have an additional so-called *g-block*, containing at least 18 elements with partially filled g-orbitals in each period.

Periodic Table Presentation:02

Precursors, cocursors and reinforcers of Mendeleev's Periodic Table

Harish Chandra Rai

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Abstract: The year 2019 marks the 150th anniversary of the birth of one of the most famous table of all time, "Periodic Table of Chemical Elements". The Periodic Table that was introduced in 1869 by Mendeleev was a monumental achievement- a wonderful mneumonic and a tool that serves to organize the whole of chemistry. The table is not outcome of the efforts of Mendeleev alone but a large number of scientists were precursors, cocursors and reinforcers of his periodic law. In the present talk I would like to highlight contributions of these scientists many of whose name did not catch the attention of the world. The notable amongst those starts from Dobereiner, Gladstone, Cooke, Odling, Lenssen, Boyle, Priestley, Davy, Faraday, Gmelin, de Chancourtois, Lother Meyer, Newland, Ramsay and Rayleigh, Thomson, Rutherford, Moseley, Bohr, Summerfield, Segre, Frankland, Lockeyer, Travers, Owen, Greger, Nilson, Del Rio, Vauquelin, Brandt, Stromeyer, Gadolin, Ekeberg, Wolaston, Mosander, de Broglie, Schrodinger, Planck, Heisenberg, Seaborg, Ghiorso, Oganessian, Flerov, Penzias, Wilson, Peebles, Goodenogh, Pykko, Poliakoff and Eric Scerri. I would also discuss the utility of lightest metal lithium which is the most useful element.

Key Note Address

Keynote address: 01

Chemistry of Pb(II) in Light Emitting Perovskite Nanocrystals

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Abstract: Unless one measures one cannot believe; the same was seen in perovskite nanocrystals. Simply connecting Pb-halide octahedras with specific cations at the lattice, all three prominent colors Red, Blue and Green could result near unity photoluminescence quantum yield. However, several sensitive issues related to the crystal chemist are associated to control this unique photoluminescence property. Similar, what one believes in classical mechanism of crystal growths in chalcogenide nanocrystals; all do not follow the same principles in making these nanocrystals in reaction flask. Lots of fun during synthesis of these colorful nanocrystals and also very much excitements seeing these crystal iunder microscope. This talk would focus on some critical issues related to brightening these nanocrystals, defect states, shape manipulations and doping in perovskite nanocrystals.

Keynote address: 02

Emerging Facets of Nitrogen Centered Radicals

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Abstract: Radicals are generated via cleavage of *tert*-butyl nitrite (TBN), organic peroxides, or using photo-catalysts, which in turn creates nitrogen centered radicals. If placed suitable the *N*-radical can trigger cascade cyclization in *o*-alkynylated *N*,*N*,-dialkylamines leading to 3-aroylindoles.[1] The higher propensity of C□N over C□S bond forming ability has been demonstrated through formal C-H functionalization during the construction of 4,5-disubstituted 1,2,4-triazole-3-thiones from semicarbazides.[2] Intramolecular C-N bond formation via cross-dehydrogenative coupling (CDC) of aryl ethers and tetrazoles have been accomplished using TBAI/TBHP with a high level of regioselectivity for substrates possessing multiple sp^3 C-H bond adjacent to the ethereal oxygen.[3]

The reagent tert-butyl nitrite (TBN) is emerging as a versatile synthons in organic synthesis.[4a] TBN serves as a “N□O” synthon during the construction of isoxazolines from terminal aryl alkenes[4b] and as a “N1” synthon in the construction of imidazo[1,2-a]quinolines.[4c] Interestingly, TBN serves the dual role of “N1” and “N-O” synthon in the construction of 1,2,4-oxaziazole-5(4*H*)-ones from terminal aryl alkenes.[4d]A visible-light-mediated concomitant C3 oxidation and C2 amination of indoles has been achieved at room temperature using an Ir (III) photocatalyst.[5]

A Bu_4NI-catalyzed regioselective *N*$_2$-methylation, *N*$_2$-alkylation and *N*$_2$-arylation of tetrazoles have been achieved using *tert*-butyl hydroperoxide (TBHP) as the methyl, alkyl diacyl peroxides as the primary alkyl, alkyl peresters as the secondary and tertiary alkyls and aryl diacyl peroxides as the arylating sources. Based on DFT calculations, it was found that spin density, transition state barriers and thermodynamic stability of the products play essentials roles.[6]

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Invited Lectures

Invited Lecture:01

Generating white-light emission from a single nano-assembly with its potential application in the detection of alkaline phosphatase activity in biological samples

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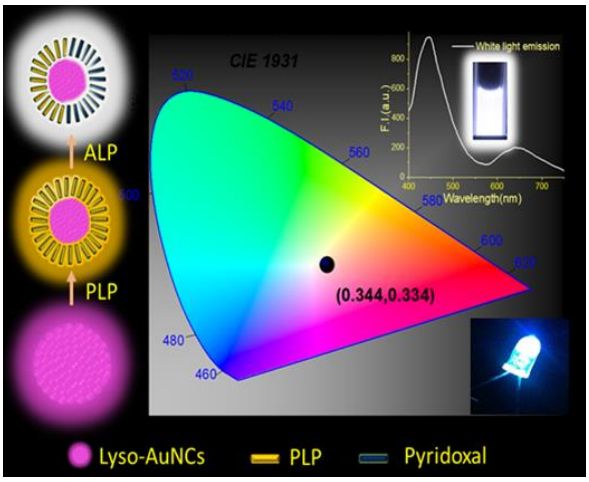
Abstract: The fluorescent dyed, optically active nanomaterials, polymers and nanoclusters are extensively studied for the generation of white-light emission owing to their potential use in lighting devices and display systems. Also, the fluorescent active molecular/nano systems are applied for theselective, sensitive and cost-effective detection of various toxic and bioactive analytes.[1] In this presentation, the designing of two novel highly selective, sensitive and cost-effective bioassays to detect alkaline phosphatase (ALP) activity using the lysozyme-stabilized and ovalbumin-stabilized fluorescent gold nanoclusters conjugated with the vitamin B6 cofactor pyridoxal 5'-phosphate (PLP) as the monophosphate ester substrate will be discussed. The cofactor PLP was conjugated with the red-emitting nanoclusters to obtain the probes*via* forming imine linkage between the $–NH_2$ group present in the coated lysozyme/ovalbumin and the -CHO group of PLP. At pH = 10.08, with the addition of ALP to the solution of PLP conjugated nanoclusters catalyzes the hydrolysis of PLP and converted in to pyridoxal, which produced a distinct ratiometric fluorescence response and the fluorescent colour turned to pale-white. The fluorescence spectral changes of the probes allowed to detect ALP activity selectively in various biological environmental samples. Further, pure white-light emitting nano-assembly was developed by conjugating optimized amounts of both PLP and pyridoxal over the surface of lysozyme-stabilized and ovalbumin-stabilized fluorescent gold nanoclusters.



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Invited Lecture:02

Designing of Nano-biomaterials for Therapeutic Applications

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Abstract:

Nano-biomaterials are categorized on the basis of their different chemical, functional, structural dimension**,** and architecture. Designing of advanced nano-biomaterials with outstanding therapeutic potential are of paramount importance in tissue engineering and drug delivery applications. This talk will discuss on utilization of nano-biomaterials in combination with laser for targeted controlled delivery of different biomolecules in to various cell lines. Nanographene functionalized with hydrophobic aromatic drugs and organic fluorophores were delivered to living cells by using laser for controlled targeted delivery and bioimaging applications. The stability and release efficacy of different drug delivery nanocarrier systems in extracellular medium will be discussed in detail. For macroscale drug delivery systems transport the nanocarrier loaded drug to the targeted site and control the release via laser or by degradation of polymer backbone. Furthermore, in recent years, it has been observed that the bacterial resistance develops faster than invention of new antibiotics. There is an urgent need to design alternative anti-microbials to replace existing antibiotics for treating a whole spectrum of bacterial diseases. To overcome this problem worldwide bacteriophage-based therapeutics appears to be a potential alternative. Bacteriophage functionalized with nanocarriers to explore the antibacterial and biofilm removal potential under laser irradiation will be discussed. The development of cationic polymer systems for enhancing antimicrobial and mineralization ability for tissue engineering applications will be outlined. Another

important development in the field of tissue engineering so far has been the utilization of magnetized nano-biomaterials, which involves the utilization of biopolymers and magnetic nanoparticle, featuring magnetic gradients for therapeutic applications.

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Award Presentations

Prof. R.C. Tripathy Memorial Award Presentation (Outside the State)

Porous Crystalline Frameworks towards Molecular Storage, Separation and Solar to Chemical Energy Conversion

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Abstract: Porous crystalline frameworks (PCFs) such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) are gaining increasing attention as new age materials due to their diverse practical applications in gas storage, separation, catalysis, sensing etc.[1] Despite such advancement, the chemical stability and synthetic difficulty are the two major challenges, which hinder their applicability. Moreover, storage, separations and catalytic conversion of gases to value added chemicals are becoming very important for many industrial applications. Although, PCFs have characteristics to being a good candidate for gas separation and photocatalysis, however, they are scarcely explored. Therefore, easy and scalable methods to synthesize these porous materials and their application as membrane materials for gas separation and photocatalytic fuel production remains a key challenge. In our research, we emphasize on simple design and easy synthesis of chemically stable MOFs and COFs;[2] their polymer composite membranes to enhance gas separation performance[3] and engineering them for solar-driven renewable fuel production[4].

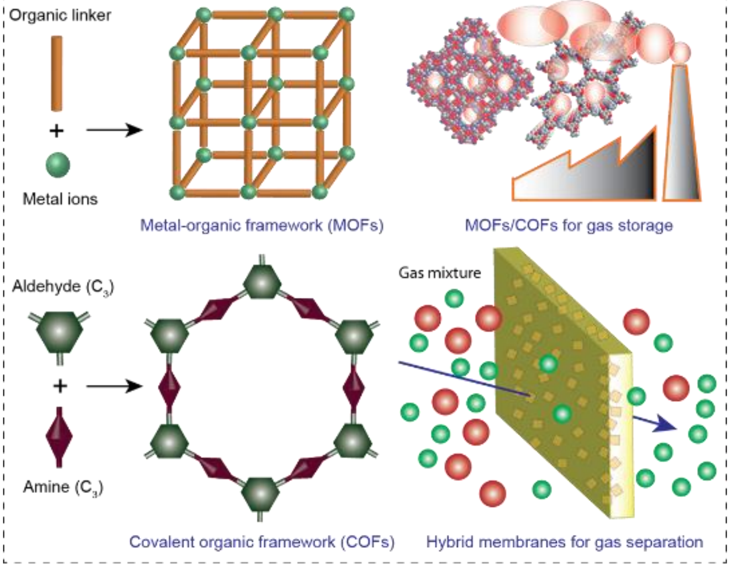

Figure 1:*Advanced Porous Materials for Gas Storage and Separation.*

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Prof. Dayanidhi Patnaik Memorial Award Presentation

Impact of Bone Extracellular Matrix Mineral based Nanoparticles on Structure and Stability of purified Bone Morphogenetic Protein–2 (BMP–2)

Monidipa Konar, Jitendra Kumar Sahoo and Harekrushna Sahoo*
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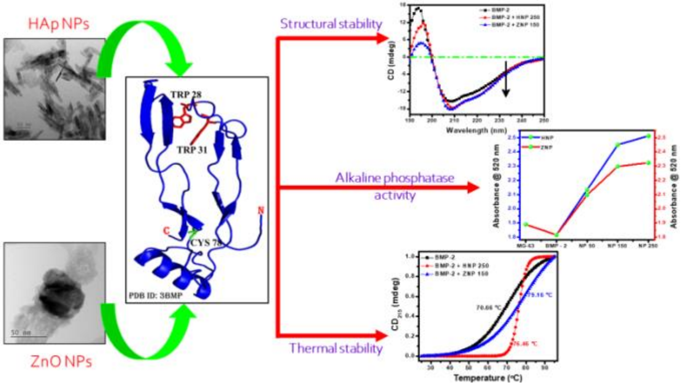
Abstract: Bone morphogenetic protein–2 (BMP–2) is an osteoinductive protein, which has been overexpressed, refolded and purified by using heparin affinity chromatography. Refolding of BMP–2 was based on urea gradient dialysis. The main objective of the present work is to unravel the impact of the inorganic minerals of bone extracellular matrix on conformation, stability and activity of BMP–2. We tried to elucidate the interaction of the bone matrix minerals in the form of nanoparticles with the osteoinductive protein. We chose hydroxyapatite nanoparticles (HAp NPs) which is the most abundant bone mineral and the other being a trace mineral in our bones i.e., zinc oxide nanoparticles (ZnO NPs) as the potential nanoparticles for this study. The isolated protein is found to be a β- sheet type with melting temperature being approximately 70.66 ˚C. Upon interaction with HAp NPs and ZnO NPs, the absorbance and the fluorescence intensity indicates the interaction with the protein as there was an upsurge in both the cases. Circular Dichroism (CD) spectroscopy revealed that ZnO NPs are having more dominant secondary structure and thermal stabilizing effect as compared to HAp NPs. Alkaline phosphatase activity confirmed the positive impact of the NPs on biological activity of BMP–2.



Prof. G.B. Behera Best Ph.D Thesis Award Presentation

High Dielectric Constant Polymer Composite Materials: A Potential Candidate of Energy Storage Devices

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Abstract: The interest of polymer nanocomposite research is growing day by day due to its wide range of potential applications. To have an idea of polymeric composites of higher dielectric strength and minimized loss, the properties are evaluated and the composites were prepared by using surface functionalized ceramic/carbon particles with various surface treating agents by solution casting technique. This study suggested strong interaction between particles and the polymer matrix, which played a key role for the improvement of the dielectric properties. The dielectric measurement results showed that the presence of surface functionalized ceramic/carbon particles enhanced the dielectric constant and relatively reduced the dielectric loss values as compared to that of untreated particles. The AC electrical conductivity of such composites was relatively high than that of the untreated one. Furthermore, the addition of surface treating agents results in enrichment of interfacial area which tightly bounded by the polymer matrix and thus responsible for the enhancement of dielectric properties. Moreover, our findings can be extended to carbon based composite material. In addition, the interfacial interaction governed by the surface treating agents play a greater role for making dielectric materials of choice for energy storage capacitors and other electronic devices.

Key words: Polymer, Nanocomposites, Surface treating agents

Kulamani Das Memorial Award Presentation

Reduced Graphene Oxide-$CuFe_2O_4$Nanocomposite: A Highly Sensitive Room Temperature NH_3 Gas Sensor

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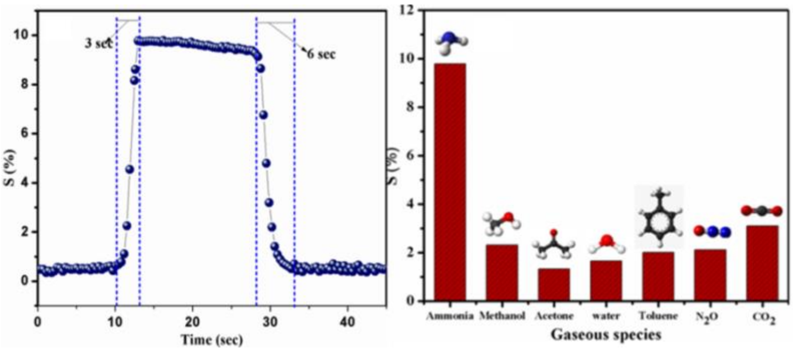
Abstract: Reduced graphene oxide (rGO) has received increasing attention since its discovery due to its variety of applications in the field of science like catalysis, sensing, drug delivery and hydrogen storage [1, 2]. The availability of oxygen-containing functional groups on the rGO sheets makes them suitable to modify with a wide range of organic and inorganic materials in covalent or non-covalent approaches to further enhance its properties [3]. Towards this objective, the present work presents a successful synthesis of $CuFe_2O_4$ nanoparticle doped rGO composite (rGO-$CuFe_2O_4$) via solution combustion method and use of this material as solid state gas sensor material. The nanocomposite was thoroughly

characterized by various sophisticated techniques such as FTIR, XRD, XPS, Raman, HRTEM with EDS mapping and TGA techniques. XRD reveals the successful formation of CuF_2O_4 structure, further supported by XPS study, which reveals the chemical environment of rGO modified by $CuFe_2O_4$ structure. High resolution transmission electron microscope (HRTEM) analysis demonstrated that the $CuFe_2O_4$ nanoparticles are uniformly distributed on rGO surface. Later on, the composite was used as a highly sensitive and active room temperature NH_3 gas sensor. The as-prepared nanocomposite acts as a very sensitive (response: 2.3%) sensor for NH_3 gas even at a very low NH_3 concentration (5 ppm). The sensing conditions were optimized by changing different parameters such as material loading (rGO:$CuFe_2O_4$), concentration of NH_3 gas and also different oxidizing and reducing organic vapours. The sensor shows very fast response time (3sec) and recovery time (6sec) towards ammonia as compare to other available sensors. Later on, the reusability and stability of the sensor were also studied for 45 days and it was found that our sensor shows response (9.3%) with respect to initial response (9.7%) for a concentration of 50 ppm of ammonia with a minimal loss of its sensing activity.



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Prof. R.C. Tripathy Memorial Award Presentation (Inside the State)

Versatile Access to Bioactive N-heterocycles

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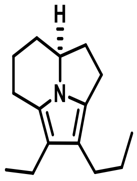
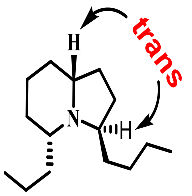
Abstract: New cases of cancer emerge in high rate, which pose challenges for chemist and biologists to fight cancer and other deadly diseases. Design and synthesis of new efficient drugs is a challenge to drug development due to several factors including drug resistances. N-Heterocycles, which are widely distributed in nature, have better oral absorption, bio-availability and displays wide array of biological activities and play very important role in metabolic activities. N-heterocycles constitute a major component in the existing anticancer

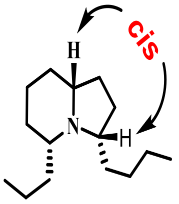
drugs. Indolizidine and isoquinoline molecules constitute such important classes of N-heterocycles having wide spectrum of biological activities. Indolizidine, isoquinoline compounds show various important bioactivities importantly anticancer, antimalaria among others. Total synthesis of Indolizidine natural products and isoquinoline derivatives have been successful by simple, versatile approach developed in the group could be useful in scaling up multi-gram batch in the drug discovery programme.



Myrmicarin 217



(-)-indolizidine 223AB



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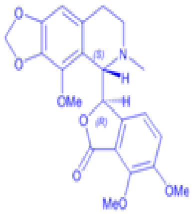

(*S*,*R*)-Noscapine

Prof. Donald S. Matteson and Prof. P. K. Jesthi Award Presentation

Excited State Dynamics of Energy Harvesting Iridium Complexes

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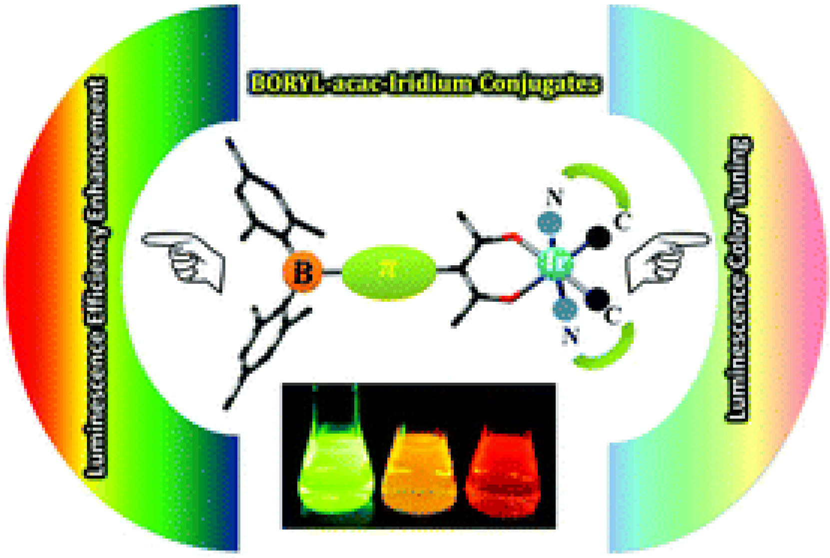
Abstract: Phosphorescent organometallic compounds have attracted a lot of attention owing to their potential applications optoelectronics and device fabrication. Studies revealed that phosphorescent cyclometalated iridium [Ir(III)] complexes have received special attention owing to their interesting optical characteristics such as high luminescence quantum yield and long lifetime.Here, we studied a series of room temperature phosphorescent compounds composed of triarylborane (TAB) and cyclometalated iridium complexes.[1] The optical characteristics such as energy of transition and luminescence quantum yield of these compounds can be conveniently fine-tuned by judiciously varying the cyclometalating ligand and the spacer between boron and iridium centers. Compounds exhibit bright phosphorescence with the emission color ranging from green to red under N_2 atmosphere and exhibit a rare type of dual emission from singlet and triplet excited states under ambient conditions. The experimental observations are well supported by the theoretical calculations. The room temperature phosphorescence features of complexes can also be exploited for device fabrications.Apart from this, I will be taking briefly on third generation of organic light emitting diodes, the thermally activated delayed fluorescence (TADF) of pure organic molecules.



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Prof. Sripati Pani Memorial Award Presentation

Iron Mineralizing Bacterioferritin A from *Mycobacterium tuberculosis* Exhibits Unique Catalase-Dps-like Dual Activities

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Abstract:*Mycobacterium tuberculosis* (*Mtb*) expresses heme binding protein nanocages, bacterioferritin A (BfrA), along with nonheme bacterioferritin B (BfrB). BfrA are unique to bacteria and like BfrB, carries out ferroxidase activity to synthesize iron oxide bio-minerals. The expression of BfrA, in the presence of BfrB, indicates that *Mtb* may utilize it for some additional purpose apart from its natural iron storage activity. During host-pathogen interaction, host secretes H_2O_2 to exterminate the pathogens; but pathogens synthesizes Dps (DNA binding protein during starvation) to detoxify H_2O_2 by utilizing it during their ferroxidase activity. Interestingly, *Mtb* lacks the gene for Dps, which protects DNA from H_2O_2, induced oxidative cleavage. Therefore, the current work investigates the kinetics of O_2/H_2O_2 dependent rapid ferroxidase reaction and DNA protection activity of recombinant *Mtb* BfrA. Ferroxidase activity of *Mtb* BfrA was found to proceed *via* the formation of a transient intermediate and exhibited sigmoidal behavior, with increasing substrate concentration, indicating the existence of cooperativity phenomenon similar to multi-subunit proteins. *Mtb* BfrA protected plasmid DNA from Fenton reagents (Fe^{2+} and H_2O_2), similar to Dps, by forming BfrA-DNA complexes. Moreover, *Mtb* BfrA exhibited catalase-like activity

by an unknown mechanism, which gets inhibited in the presence of NaN_3 and NaCN. Thereby, *Mtb* BfrA executes multiple functions (ferroxidase, catalase and Dps-like activities) (**Fig. 1**) to cope up with the host generated oxidative stress and to promote pathogenesis.

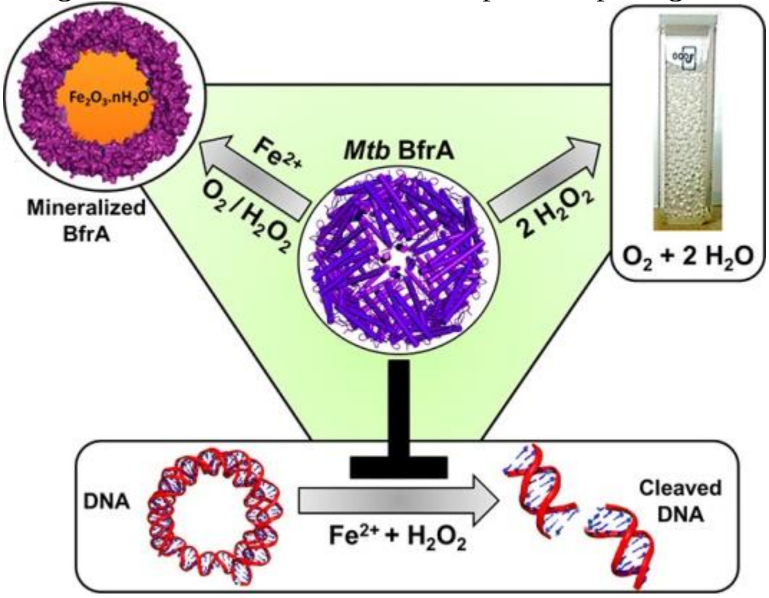

Figure 1:*Heme binding Bacterioferritin A (BfrA) Protein Nanocages from Mycobacterium tuberculosis (Mtb) Mimics Catalase (O_2 Evolution) and Dps (DNA Protection), in addition to Its Rapid Iron Mineralization Activity.*