

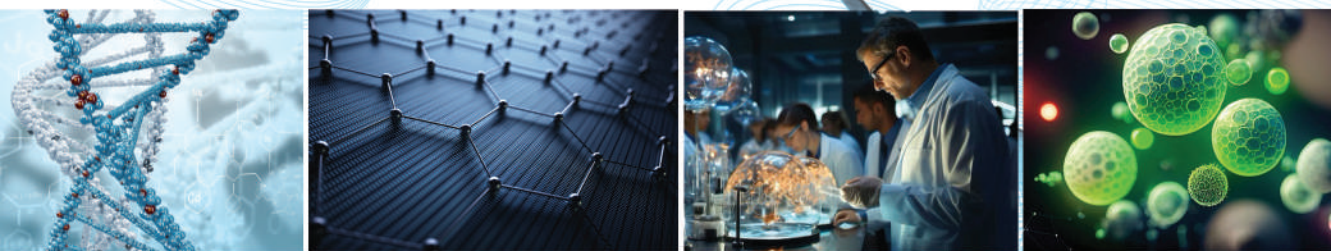
National Seminar

# FRONTIERS IN CHEMICAL SCIENCES

## FCS 2024

13-15 February, 2024

**BOOK OF ABSTRACTS**



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# FCS 2024

National Seminar

## FRONTIERS IN CHEMICAL SCIENCES

February 13<sup>th</sup> - 15<sup>th</sup>, 2024

# BOOK OF ABSTRACTS

Organized by



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## Message

Science is, in a sense, a realm of collective human activity too. Hence, it is inherent in its nature that its practitioners look forward to gathering to exchange information and knowledge. Universities, as centres of knowledge production and dissemination, are therefore duty-bound to set up and encourage these gatherings.

True to this spirit, the Department of Chemistry, in the University of Calicut has been arranging an event named '**Frontiers in Chemical Sciences (FCS)**' which has grown into a highly noticed annual Symposium in the National level. It brings together leaders of various areas of Chemical Sciences, emerging investigators, young researchers and students under its umbrella. The free discussions and interactions that naturally follow have been highly helpful for the growth of the field, young researchers and students. As a Physicist, I have also thoroughly enjoyed attending a few technical sessions in previous editions of FCS.

Continuing this tradition, FCS 2024 is being organised from 13<sup>th</sup> to 15<sup>th</sup> February by the Department of Chemistry. I am sure that the event will be a memorable one for all its attendees. I am happy to welcome the participants of FCS 2024 to the University of Calicut. I wish FCS 2024 all success.



**Prof. (Dr.) M. K. Jayaraj**  
Vice Chancellor



Dr. M. Nasser  
Pro-Vice Chancellor

UNIVERSITY OF CALICUT

Dated: 09.02.2024

## MESSAGE

The vehicles for the onward march of Science and Technology are mostly forged in laboratories, but its direction and speed are essentially dictated in the discussions and interactions of scientists outside the lab. Therefore, it is essential that scientists of all types, meet regularly, exchange ideas, share concerns, chalk out plans for future endeavours and define larger goals for their areas. Scientific conferences and symposia evolved exactly for these reasons.

This important tradition is being continued by the Department of Chemistry in the form of an annual national seminar, Frontiers in Chemical Sciences (FCS), which has become a highly visible event over the years. It has been attracting leaders of Indian Chemistry to the University of Calicut. Previous editions of FCS have led to many fruitful collaborations, student exchanges and birth of many new ideas.

I am sure that this year's edition of FCS that is being organised by the Department of Chemistry on 13-15 February will build on its illustrious legacy. I wish FCS 2024 all success.



**Dr. M. Nasser,**  
**Pro-Vice Chancellor.**

## Foreword

Chemical Science, has been traditionally called the Central Science, due to its relative position with respect to the Physical and Biological counterparts. The centrality creates overlaps with neighbouring realms that dissipate the borders and gives rise to new areas of common activity. Thus, it is essential that these *Frontiers* are identified from time to time by practising chemists for marking areas of high activity, charting new courses and unearthing new concepts and products. The only way to make this possible is by bringing the practitioners of the art together, promoting interactions and exchange of ideas. Scientific meetings and symposia aim nothing less.

The Department of Chemistry, University of Calicut has been organising a National Symposium, *Frontiers in Chemical Sciences (FCS)* every year with the objectives stated above. Over the years, FCS has grown into a highly sought-after event that witnessed stories of pathbreaking discoveries, provided fertile ground for nurturing successful collaborations and enlightened and inspired a number of young researchers. The Department proudly continues this cherished tradition in the form of FCS-2024 during February 13-15.

The Department of Chemistry is happy to present to you the compilation of contributions that enriched FCS-2024 in the form of this *Book of Abstracts*. The reader will find abstracts of 1 keynote address, 16 invited lectures, 4 short invited lectures, 11 oral presentations and 26 poster presentations that address diverse areas of Chemical Sciences. The enormous efforts to collect, compile and publish this book of abstracts were made by the abstract committee members, editorial board members, other faculty members, research scholars and staff of the Department. We hope that it will find a permanent place in your memory and bookshelf.

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## **A Scalable Recipe for Self-Forming Ag-Based Neuromorphic Devices**

**Giridhar U. Kulkarni<sup>a\*</sup>**

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The human brain, comprising nearly a hundred billion neurons with several order higher number of synapses, accomplishes massive parallel processing and unmatched cognitive actions. Inspired by this, efforts are being made worldwide to develop artificial neural networks to mimic intelligence with the help of complex algorithms incorporated on the currently available high-speed computational platforms. However, solving intricate real-world problems which a biological brain routinely deals with in real time, have posed tremendous challenges even to state-of-the-art computers. A biological synaptic junction, unlike the present day computing units, appears to handle both processing and memory parallelly, an aspect closely linked to its ability to change with the circumstance, termed neuroplasticity. While neuroplasticity in relation to memory and processing is still being investigated, efforts in the literature are increasingly based on mimicking different levels of neuroplasticity using artificial synaptic devices.

The presentation covers the literature on this topic with emphasis on self-forming device recipes. A self-formed labyrinth structure of Ag, mimicking neuronal bodies and axonal network connectivity at least remotely, has been explored in the laboratory and the outcome of the study will be described. This interesting device architecture enabled us to emulate using voltage spike signals, basic to complex synaptic activities, importantly, without the aid of external circuitry. Besides STP and LTP interestingly, behaviours akin to human intelligence have been realised. Another important feature is linear updating of the synaptic weight which serves for in-memory computation.



# INVITED LECTURES

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## **The Science of Designing a Good Life**

**Suresh Das<sup>a\*</sup>**

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**Keywords:** Passion, Flow, Ethics, Purpose

All of us would like to have a good life, but give very little thought to what we mean by it. We use the word design, meaning to create or construct according to a plan, for many simple things in life as also in developing complex technologies. Is it possible however to use the word in the context of life itself? Several philosophers, psychologists and other thinkers have endeavored to address what it takes in order to succeed in the game of life. Is it survival of the fittest? Do we compete or cooperate, give or take? Studies have shown that behaviors such as generosity, morality, conscience and empathy required for the success of groups are also the traits that are beneficial for individual success. This lecture will focus on some of these issues.

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## Stimuli Responsive Supramolecular Materials of Self-assembled Bodipys

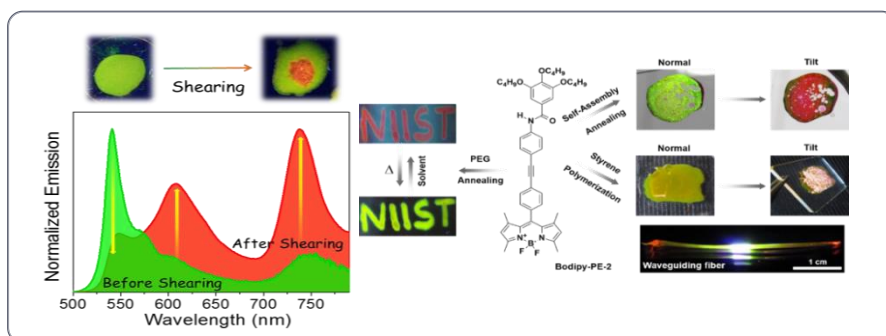
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**Keywords:** Stimuli responsive materials, Supramolecular chemistry, Self-assembly, Bodipy

Supramolecular soft materials derived from chromophore-linked  $\pi$ -systems have generated significant attention because of their interesting stimuli responsive physicochemical properties, particularly optical properties.<sup>1,2</sup> Since, morphological features of chromophore assemblies play important roles in the optical behavior, any attempt to control the hierarchical structures of molecular assemblies is of considerable significance. Among different chromophore-linked  $\pi$ -systems, 4,4-Difluoro-4-bora-3a-4a-diaza-s-indacene (Bodipy) is a preferred chromophore due to its synthetic accessibility and tunable emission behavior. Recently, we have reported a few Bodipy-linked phenyleneethynylene (Bodipy-PE) derivatives and studied their self-assembly behavior and the associated optical property changes.<sup>3-5</sup> Rational design of molecular structures, allowed us to obtain mechanoresponsive and photonic materials with NIR emission and angle dependent optical reflection, respectively (see figures below) wherein noncovalent interactions play an important role. Details of these studies will be discussed.



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## **NMR from a High-Field and a Low-Field Perspective**

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**Keywords:** Solid-state NMR, Zero-field NMR, magic-angle spinning, ZULF

We will highlight the advances made in solid-state nuclear magnetic resonance (NMR) spectroscopy that has enabled its applications in a variety of fields, ranging from small molecules to biomolecules to batteries to solar cells and many more. Representative applications from some of these will be shown that mark the potential of the method. Besides these, an overview will be shown of the emerging method of zero-ultra-field NMR (ZULF) method in the context of magnetometry and spin metrology.



**IL 04****From Sunlight to Electricity - The Fabrication of an Organic Solar Cell****K. R. Haridas<sup>a\*</sup>***<sup>a</sup>School of Chemical Sciences, Kannur university, Kannur, Kerala, India.**\*krharidas2001@gmail.com*

A solar cell is an electronic device that converts the energy of light directly into electricity by means of the photovoltaic effect. The electricity produced by solar cell depends on various parameters such as light wavelength, light intensity, light incident angle, surface area of solar cell, temperature of solar cells and type of solar cell. Organic solar cells are made of thin layers of organic materials with thickness in the 100 nm range. The motivation for using organic dyes is to replace the expensive silicon in conventional photovoltaics and to apply simple production techniques. The molecules used in organic solar cells are solution-processable at high throughput and are cheap, resulting in low production costs to fabricate a large volume. Compared to silicon-based devices, polymer solar cells are lightweight (which is important for small autonomous sensors), potentially disposable and inexpensive to fabricate (sometimes using printed electronics), flexible, customizable on the molecular level and potentially have less adverse environmental impact. The main components of an organic solar cell consisted of 1) A conducting electrode coated over a hard substrate, 2) Nanoporous semiconductor of comparable bandwidth, 3) a sensitized dye 4) a hole transporting material and 5) a counter electrode. The synthesis and characterization of dye, nanoporous and hole transporting materials are depicted. After the optimization of the material characteristics, the organic solar cells are fabricated. The methods of fabrication of an organic solar cell are sketched. A thorough study of the failure in processing which depicted on the efficiency is also under study.

## Magnetic Nanoparticle Clusters for Environmental Remediation and Biomedical Applications

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**Keywords:** Magnetic nanoparticle clusters, magnetic hyperthermia, drug delivery

Magnetic nanoparticle clusters where numerous smaller-sized nanocrystals bound together are advantageous for environmental remediation and biomedical applications, because of their superior saturation magnetization values which will enable them to retort fast to an external magnetic field.<sup>1</sup> Furthermore, these secondary structures can retain the superparamagnetic characteristics of the constituting primary nanocrystals even if the overall nanocluster size exceeds the critical size for superparamagnetic to ferromagnetic transition. Magnetic nanoparticle clusters of different sizes can be synthesized by a facile solvothermal approach and the primary nanocrystallite size can be tuned by varying the surfactant concentration during the solvothermal treatment.<sup>2</sup> The radio frequency alternating magnetic field-induced heating studies indicated that as-synthesized magnetic nanoclusters are promising candidates for magnetic fluid hyperthermia applications. The specific absorption rates increased linearly with the square of the external field amplitudes, which is in accordance with the linear response theory.<sup>3</sup> Magnetic nanoparticle clusters having mesoporous structures are ideal drug carriers since they can allow fast diffusion, adsorption and subsequent release of drug molecules through their three-dimensional pores.<sup>4</sup> Magnetic nanoparticle clusters can be combined with 2D nanomaterials such as graphene oxide (GO) which can yield new functional hybrid materials that will combine the high adsorption capability of GO and the separation advantage of magnetic nanomaterials. These nanohybrids hold great potential as an efficient and recyclable adsorbent for the removal of dye pollutants for environmental remediation applications.<sup>5</sup>

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## IL 06

### Role of Radioisotopes in Healthcare

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**Keywords:** Radioisotopes, Radiations, Diagnosis, Therapy, Cancer

While the use of nuclear power for generating electricity is common knowledge, their prominence through the use of radioisotopes in modern day healthcare is not obvious. Though radioisotopes are present in nature, man-made radioisotopes with suitable nuclear properties can be used for non-invasive evaluation of organ function and diagnosis or therapy of diseases like cancer. Compared to other non-invasive imaging modalities such as coaxial tomography (CT) and magnetic resonance imaging (MRI), nuclear medicine, the modality which uses radiations emitted by radioisotopes, is much more sensitive. Radiopharmaceuticals, target specific biomolecules tagged with suitable radioisotopes, form the backbone of nuclear medicine. Today, positron emission tomography using [<sup>18</sup>F]-fluorodeoxyglucose ([<sup>18</sup>F]-FDG) is a frontline diagnostic tool for cancer diagnosis.<sup>1</sup> Beta particle emitting therapeutic radiopharmaceutical [<sup>177</sup>Lu]-DOTATATE<sup>2</sup> and [<sup>177</sup>Lu]-PSMA-617<sup>3</sup> has provided a means for effective clinical management of neuroendocrine cancers and prostate cancer, respectively. Currently, Chemoradiotherapy, a synergistic combination of chemotherapeutics and radiation, is being actively explored to enhance the clinical management of cancer. Often, nanoparticles are used as platforms to develop chemoradiotherapy agents, which provides options for simultaneous loading of the chemotherapy drug and the radioisotope for delivering therapeutic dose to the cancer tissue. Thus material scientists has an important role in providing biocompatible nano-platforms to develop such agents. The field of nuclear medicine offers an opportunity for material scientists, radiochemists and radiopharmaceutical chemists to work together to bring a significant change in terms of providing an affordable and effective healthcare to our society. The talk will cover basic concepts and different approaches for preparing target specific radiopharmaceuticals for diagnosis and therapy of cancer.

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## Interaction of Radiation with Molecules and Matter: Applications and Opportunities

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**Keywords:** Radiation and Photochemistry, Molecular Assemblies, Cucurbituril-functionalized Nanocomposites, Hydrogen Production

This presentation would provide a broad overview of interaction of high-energy and low-energy photons with molecules/matter and showcase the technological advantages and wide-ranging applications of radiation and photochemistry in the present scenario. The excitation and ionization due to the energy absorption/deposition, particularly in aqueous based chemical systems, leads to the generation of excited states, free radicals and their subsequent chemical reactions. These excited states and radical species are channelled to have specific interactions with the molecules of interest, either in chemical systems or in complex biological environment to exploit their utility in medical applications, especially in diagnostic and therapy for cancer. The talk will also cover the meticulous control of the weak non covalent interactions present in the molecular assemblies on exposure to low energy photons in the UV-Vis region. Apart from their directed reactions to generate reactive radical anions in confined nanocavity, the noncovalent interactions has been also demonstrated for the enhanced production of green hydrogen from the hydrolysis of boron-based hydrides, better by the cucurbit[7]uril-functionalized metal-alloy nanocomposites. The cavitation strategy has also been used for the cooperative enhancement of antibacterial activity of drugs and several molecular assemblies have been tested for probing mechanisms that underlie human neurodegenerative diseases in living model organisms such as *Drosophila melanogaster* fly, and to address fibril-induced neurodegenerative disorders.

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**IL 08**
**Carbon Nanotube for Affordable Wearable Devices**
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**Keywords:** Flexible Electronics, Multiwalled Carbon Nanotube, Piezoresistive Strain Sensor

Multiwalled carbon nanotube (MWCNT) by virtue of its inherent mechanical stability, oxidation inhibition, and intrinsic electron mobility, is now evolved as the cheaper solution to some of the burning challenges in flexible electronics. This talk outlines our efforts to develop two cost effective wearable devices employing MWCNT.<sup>1</sup>

In the first work package, an all printed flexible, energy-efficient wearable heater was fabricated using a resistive ink principally made of MWCNT. Herein, a systematic investigation on employing PEDOT:PSS as an effective binder and dispersant for affordable conductive ink manufacturing was carried out. Screen printable room temperature curing formulation made of MWCNT and PEDOT:PSS is being reported for the first time. The ink's enhanced stability is contributed by the  $\pi$ - $\pi$  interaction between MWCNT and PEDOT:PSS. The printed conductive traces showed a sheet resistance of  $51.31 \pm 0.25 \Omega/\square$  on Mylar substrate, ideal for flexible heater applications. The screen printed flexible heater based on MWCNT-PEDOT:PSS nanocomposite has impressive energy efficiency and thermal stability, generating a peak temperature of 136 °C at the expense of only 0.137 W/cm<sup>2</sup>.<sup>2</sup>

In the second work package, silver nanoparticles were decorated on the surface of MWCNT. Employing this Ag@MWCNT, a multifunctional room temperature curable conductive ink was developed, with PEDOT: PSS as the conductive binder. The versatility of the ink for developing functional elements for printed electronics was demonstrated by fabricating prototypes of a wearable strain sensor, a smart glove, a wearable heater, and a wearable breath sensor. The printed strain sensor exhibited a massive sensing range for wearable applications, including an impressive 1332% normalized resistance change under a maximum stretchability of 23% with superior cyclic stability up to 10000 cycles. The sensor also exhibited an impeccable gauge factor of 142 for a 5% strain (59 for 23%). Further, the sensor was integrated into a smart glove that could flawlessly replicate a human finger's gestures with a minimal response time of 225-370 ms. Piezoresistive vibration sensors were also fabricated by printing the ink on Mylar, which was employed to fabricate a smart mask and a smart wearable patch to monitor variations in human respiratory and pulmonary cycles. Finally, an energy-efficient flexible heater was fabricated using the developed ink. The heater could generate a uniform temperature distribution of 130 °C at the expense of only 393 mW/cm<sup>2</sup> and require a minimum response time of 20 s.<sup>3</sup> In brief, through a meticulous choice of organic vehicles, MWCNT based ink is proved to be ideal for realizing versatile printed devices for future wearable applications.

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## **Electrochemical production of Ammonia: Stakes and Challenges**

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Ammonia (NH<sub>3</sub>) is the second-highest-produced chemical commodity, with an annual production that hovers around 240 million tonnes. It is currently produced on a large scale using the conventional Haber-Bosch process, which requires high temperature and high pressure and consumes about 2% of the world's energy supply. Electrochemical nitrogen (ENR) reduction and nitrate reduction (NO<sub>3</sub>RR) using renewable energy sources serves as a sustainable route to mitigate the environmental problem.

In my talk, I will highlight the challenges associated with ENR in aqueous media and highlight the need for standardized protocols to accurately quantify NH<sub>3</sub> at sub-ppm concentrations, free from false-positives. Furthermore, I will discuss electrochemical nitrate reduction (NO<sub>3</sub>RR) as a promising pathway for electrochemical NH<sub>3</sub> production.

**IL 10**
**N-Heterocyclic Carbene (NHC)-Catalyzed Synthesis of C-N, C-O and N-N Axially Chiral Molecules**
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N-Heterocyclic carbene (NHC)-catalyzed umpolung of aldehydes is widely used for the unconventional access to target molecules.<sup>1</sup> Although the assembly of axially chiral C-C bonds leading to the atroposelective synthesis of biaryls and related compounds are well-known, the analogous synthesis of compounds bearing axially chiral C-Heteroatom bonds are relatively rare using NHC catalysis. We have recently reported the NHC-catalyzed atroposelective synthesis of N-aryl succinimides having an axially chiral C-N bond via the desymmetrization of N-aryl maleimides.<sup>2</sup> Moreover, we have demonstrated the NHC-catalyzed kinetic resolution of N-aryl aminomaleimides allowing the synthesis of C-N axially chiral N-aryl aminomaleimides via remote chirality control.<sup>3</sup> In addition, NHC-catalyzed selective amidation reaction leading to the atroposelective synthesis of N-N axially chiral 3-amino quinazolinones has been realized recently.<sup>4</sup> Further, we have uncovered the NHC-catalyzed synthesis of C-O axially chiral diaryl ethers via atroposelective esterification of dialdehyde-containing diaryl ethers via a desymmetrization strategy.<sup>5</sup> The details of these works will be presented.

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## **Plasticity and Yielding in Amorphous Solids**

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The mechanical response of a wide range of amorphous solids is of interest in diverse contexts, from molecular glasses, a variety of soft materials such as polymeric glasses, colloids, to granular matter including in geological contexts. Amorphous solids exhibit microscopic aspects of plastic deformation that are distinct from crystalline solids. The nature of such plasticity and the eventual yielding behavior have been investigated extensively in recent years through computer simulations and statistical mechanical approaches, which will be briefly reviewed. In particular, yielding under cyclic shear deformation has been characterized in detail in computer simulations as a sharp, discontinuous transition, which further exhibits striking dependence on the degree of annealing of the amorphous solids subjected to shear. Several of the interesting features observed in simulations are well captured by theoretical models and simulation of elasto-plastic models, while several basic questions remain. The successes and limitations of our present understanding will be summarized.



## Progress in Organic Solar Cells: Past and Future

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**Keywords:** Organic solar cells, Power conversion efficiency, Design concepts

Organic solar cells (OSCs) are one of the emerging photovoltaic (PV) technologies currently investigated as potentially low-cost renewable energy sources. Diligent work in the OSC area has pushed the achieved power conversion efficiency (PCE) bar to 20%. This is mainly fueled by introducing non-fullerene acceptors (NFA), improved device engineering, and enhanced photophysical understanding. As the OSC devices are approaching the 20% PCE milestone, they can be a potential competitor in the PV market. To make the market entry of OSC, the efficiency needs to be further improved. The external quantum efficiency, EQE is dictated by the efficiency of photon absorption ( $\varphi_{\text{abs}}$ ), exciton dissociation ( $\varphi_{\text{diss}}$ ), charge pair separation ( $\varphi_{\text{sep}}$ ), and charge extraction ( $\varphi_{\text{extr}}$ ). In this presentation, I will discuss the fundamentals of charge generation in OSC and how they differ from inorganic traditional solar cells. I will start by briefing the challenges we faced in the past and how the OSC community overcame those obstacles. Further, I will share some of our recent efforts toward understanding the physics of organic solar cells to create more charges and design rules we derived from those studies.<sup>1,2</sup>

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## Multitude Application Domains of the Supramolecular Conjugates of Calix[4]arenes

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Activity concerned with the synthesis of the conjugates of calix[n]arenes *via* organic derivatization affecting the lower rim or the upper rim or both has become routine among chemists who work on this class of supramolecules. The current literature is abundant with synthetic designs. When the advantages of these two aspects are taken into consideration, it is not impossible to develop and synthesize the conjugates of calixarenes suitable to perform specific functions. Recent developments of these by anchoring on to the solid surfaces have elevated their utility in a variety of fields. Thus, there lies a tremendous potential for properly designed and carefully tailored conjugates of calix[n]arenes to serve as materials for multitude applications and thus the influence of calixarenes has gone much beyond sensing. During the past decade, our group entered into the arena where the conjugates of calixarenes are appropriately designed and demonstrated for their cell targeting, anticancer activity, drug delivery, gene transfer, catalysis and in water purification.

We have recently designed and developed a number of conjugates of calix[4,6]arenes and studied their applications. However, in this lecture I shall focus on the outcome based on the efforts from our research group in the case of the conjugates of calix[4]arenes spanning across the past 7 to 8 years. The corresponding publications arising from our research group can be gauged from the references given in this abstract.<sup>1-11</sup> Several of these will be a part of this lecture.

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## IL 14

**Supramolecular Synthons Modulation in Crystal Engineering: A Structural Outlook****P. Venugopalan\****<sup>a</sup>Department of Chemistry, University of Calicut, Thenhipalam, Malappuram, India**\*venugopalanp@yahoo.com, venu@uoc.ac.in***Keywords:** Crystallography, Supramolecular Synthons, Self-assembly

The control of molecular organization based on specific molecular attributes is a challenge in crystal engineering. An advantageous approach to the crystal structure prediction and engineering relies on the identification and exploitation of certain patterns of association (i.e., supramolecular synthons) that are robust and recur decisively in the crystal packing. In this direction, a variety of supramolecular synthons based on O/N-H...O/N hydrogen bonds have been identified. Although the importance of weak but directional C-H...O/N hydrogen bonds has been amply exemplified, the quest for identification of new and novel synthons continues unabated as it constitutes one of the fundamental objectives of crystal engineering. In this direction, we have shown through rational design and X-ray structural analysis of large number of o-methoxy-benzaldehydes that they tend to associate in a centrosymmetric fashion akin to carboxylic acids which derive stabilization from four C-H...O hydrogen bonds. These aldehydes found to undergo self-assembly into 1-D molecular tapes and staircases.

The well-known >C=O...X interactions control the crystal packing of o-haloaromatic carboxaldehydes as revealed by the X-ray crystal structures of number of carboxaldehydes. The intramolecular C-H...X interaction causes the >C=O...X interactions to manifest in a readily recognizable pattern of association, i.e., a supramolecular synthon whose robustness is amply suggested from the isostructurality exhibited by four dichloro- and dibromo- dialdehydes. The sterically encumbered carboxylic acids derived from these aldehydes undergo helical self-assembly through weak X...X and >C-H...X interactions and this molecular organization is different from the common dimer synthon observed in carboxylic acids which is highly prominent in crystal engineering applications. It is also rationally possible to exploit these interactions in combination with steric encumbrance to induce cavity formation in the crystals which can be filled by solvents of crystallization or molecules of appropriate size and molecular shape. This can find applications in separation techniques. The weak X...X interactions can further be extended to the realm of organometallic compounds to generate ladders, 1D and 2D networks in hexa-coordinated Sn(IV) porphyrins. Details will be presented.

## Intrinsic Chirality at the Nanoscale: Exploring Ground and Excited State Optical Activity

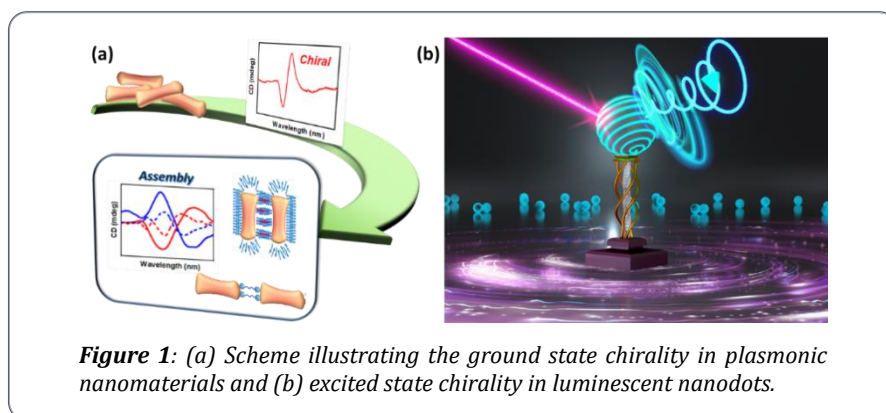
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**Keywords:** Nanoscale chirality, circular dichroism, circularly polarised luminescence, plasmonic nanomaterials

Chirality is a unique geometric property observed in nature at different hierarchical scales ranging from subatomic particles to galaxies. The field of chirality has seen a rejuvenation after the observation of optical activity in different classes of nanomaterials. Moreover, these materials have found application in the field of biosensing and light emitting devices. A combination of two techniques, namely circular dichroism (CD) and circularly polarised luminescence (CPL), helps unravel the underlying mechanism of ground and excited state chirality in these materials. Our attempts have been to fabricate chiral light absorbing as well as chiral light emitting materials adopting three different strategies. These include (i) synthesis of intrinsically chiral nanoparticles,<sup>1-3</sup> (ii) chirality induction through interaction with ligands<sup>4</sup> and (iii) the template assisted generation of chirality using a host guest approach. Our recent attempts towards synthesizing intrinsically chiral nanomaterials and understanding the mechanistic details of ground state (Figure 1a) and excited state chirality (Figure 1b) at the nanoscale will be discussed briefly.



**Figure 1:** (a) Scheme illustrating the ground state chirality in plasmonic nanomaterials and (b) excited state chirality in luminescent nanodots.

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## IL 16

### Phase Transformations and Morphology Tuning in Perovskite Nanocrystals

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**Keywords:** Phase transitions, Morphology, Perovskite nanocrystals

Organic-inorganic metal halide perovskites ( $ABX_3$ ) have been significantly explored in the past decade owing to their excellent photo-physical properties. These unique inherent features exposed them to find applications in photovoltaics, optoelectronics and catalysis.<sup>1</sup> Introduction of various cations into the framework of perovskite lattice, have been shown to improve the stability and performance *via* partial exchange with either A or B cations. However, traditional high-temperature cation exchange reactions lack control over the shape, composition, stoichiometry and crystalline habit of nanocrystals, incited exploration of low-temperature methods for precise & controllable modifications. Herein, we investigated the solution phase interaction of coinage (Au,Ag,Cu) metal ions and monovalent organic cations with cesium lead bromide ( $CsPbBr_3$ ) nanocrystal under ambient conditions. Simple addition of Au and Ag metal ions into  $CsPbBr_3$  nanocrystals induce a facile formation of metal decorated perovskite nanocrystals<sup>2,3</sup> whereas the monovalent Cu ions explicitly initiates a one-dimensional growth with a distinct phase transition, i.e., from cubic to orthorhombic. Controlled addition of organic monovalent cations allowed a reversible tuning of the dimensionality of perovskites.<sup>4</sup> The mechanistic investigation of the formation of metal-hybrid nanocrystals, phase transitions and associated morphology change is accomplished *via* structural & morphological characterisation using XRD, XPS & HRTEM analysis. In this talk, I will be discussing how tuning of the tolerance factor *via* room temperature modifications and cation exchanges in perovskite nanocrystals could play a key role in tuning morphology, dimensionality and anisotropy.

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# SHORT INVITED LECTURES

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## Quinolone-3-Carboxamide Derivatives: Design, Synthesis, and Identification of Potent Anticancer Agents

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Cancer is one of the most complex and persistent challenges that the medical field is facing. According to the International Agency for Research on Cancer (IARC), there were 19.3 million new cancer cases and nearly 10 million cancer deaths reported in 2020 worldwide. The global cancer burden is estimated to increase to 28.4 million in 2040 which is a 41% rise from 2020.<sup>1</sup> Among the different types of cancer, breast, lung, and colon cancer are the leading cause of death globally.<sup>2</sup> Therefore, highly efficient and target-specific drugs to treat various cancers with minimal/no side effects are essential globally.

Linomide, Laquinimod, Paquinimod, and Tasquinimod are quinolone-3-carboxamide derivatives. Linomide has been reported as an immune stimulant that enhances NK cell activity and macrophage cytotoxicity.<sup>3</sup> Whereas, Laquinimod and Paquinimod are approved as drugs to treat autoimmune diseases, and Tasquinimod (**IV**) is under clinical trials (Phase III) for the treatment of solid tumors.<sup>4</sup> Due to the significant importance of quinolone-3-carboxamide derivatives in the field of medicinal chemistry, twenty-eight new molecules were synthesized and evaluated for their *in vitro* anticancer activity against the colorectal cell line (HCT116), lung cell line (A549) and breast cell line (MCF7). All the compounds exhibited good activity against all three cell lines with IC<sub>50</sub> values ranging from 0.168-43.317  $\mu$ M. Among them, three potent compounds were selected to identify their mode of action. Culture morphology, autophagy evaluation, colony formation, mitochondrial, lipid droplets, nucleus evaluation, DNA damage studies, and cell cycle analysis were performed. From these experiments, it was found that the compounds have multiple mechanisms of action, including changes in cellular and nuclear morphology, disruption of mitochondrial function, lipid accumulation, DNA damage, cell cycle arrest, and ultimately induction of apoptosis. These findings suggest that the compounds may have a broad spectrum of activity against different types of cancer and could potentially be developed into effective anticancer drugs.

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## SIL 02

### Rongalite: A Multifaceted Green Reagent in Organic Synthesis

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Sodium hydroxymethanesulfinate dihydrate (SHM), commonly known as rongalite, is an industrial product with diverse applications. It serves as a bleaching agent in the dye and printing industry, functions as a reducing agent, acts as an antidote against heavy metal poisoning, and serves as an antioxidant in formulations. Additionally, it plays a role as a green reagent in organic chemistry. This versatile reagent finds use in the synthesis of various compounds, including sultines, sulfones, spirooxindoles, sulfides, thioesters, selenoesters, and allyl alcohols. Notably, it proves to be a valuable source of the C1 unit in the synthesis of 2,4,5-trisubstituted furans. Our research has introduced a novel method utilizing rongalite's multifaceted properties as a reducing agent, chemoselective reducing agent, oxidizing agent, C1 unit source, and as a dual-role agent for reducing/C1 unit in organic synthesis (Figure 1).

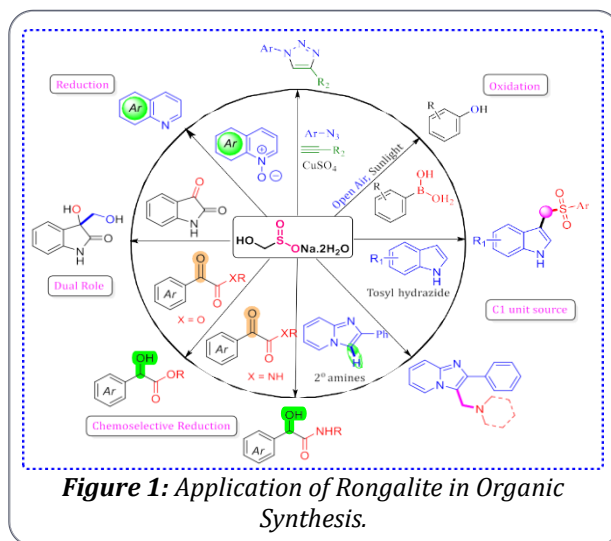


Figure 1: Application of Rongalite in Organic Synthesis.

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## SIL 03

## Design and Synthesis of Spiroheterocyclics as Potent Anticancer and Antitubercular Agents

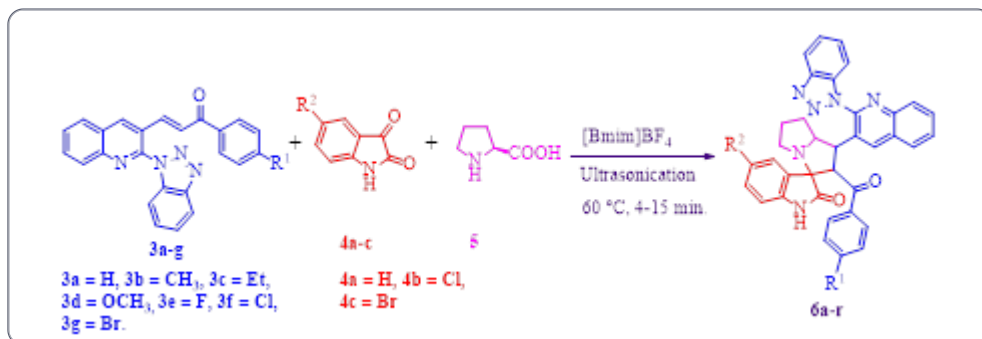
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**Keywords:** Spiroheterocyclic compounds, 1,3-dipolar cycloaddition, anti-cancer, anti-tubercular agents

The essential need for the potent anticancer and antitubercular agents with high selectivity and safety profile prompted us to synthesize a new series of spiro heterocyclics, spiro pyrrolizidines. These compounds were synthesized by one-pot multicomponent [3+2] cycloaddition reaction under reflux/ultrasonication. Further, *in vitro* anticancer and antitubercular activity were evaluated against human lung carcinoma (A549) and human cervical (HeLa S3) cancer cell lines and *Mycobacterium tuberculosis* H37Rv respectively.



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## SIL 04

### Base-Metal Catalysed Hydrofunctionalisation of Un-activated Ketones

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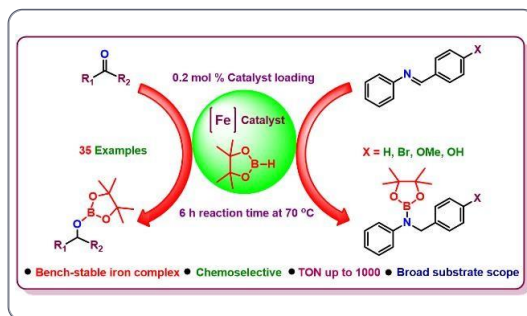
**Keywords:** Catalysis, hydrofunctionaliation, base-metals, Salen type ligands

Recent research is focusing on sustainable catalysis, moving away from precious metals towards earth-abundant transition metals such as Mn, Fe, Co, and Ni<sup>1</sup>. Base metals offer cost-effectiveness and ready availability in catalytic transformations such as hydrogenation, hydrosilylation, and hydroboration. While ligand systems like N-heterocyclic carbenes are commonly used, Salen type Schiff base ligands remain underexplored. These ligands, with a tetradentate geometry, show promise due to their facile metal coordination, tunability for steric and electronic properties, and ability to stabilize and enhance metal performance in different oxidation states. Their potential in various catalytic transformations aligns with the goal of promoting green and eco-friendly methods in industrial applications.

We have developed a series of Salen type cobalt and iron<sup>2</sup> complexes with tunable steric and electronic properties, addressing limitations in existing reports. These complexes demonstrated exceptional catalytic activity in hydrosilylation and hydroboration of ketones. The catalysts exhibited high yields, remarkable chemoselectivity, broad substrate scope (including aromatic, aliphatic, and heterocyclic ketones), and excellent atom economy under mild conditions with minimal catalyst loading (ppm level to 0.2 mol%). Notably, the catalytic system showed efficiency in gram-scale reactions, indicating its synthetic applicability. Through literature studies and control experiments, we propose plausible catalytic cycles involving active intermediate species ([Co]-H and [Fe]-H) responsible for ketone hydrosilylation and hydroboration, respectively.

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# ORAL PRESENTATIONS

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## Identification of Hla-Dr Associated Peptides Involved in Beryllium Hypersensitivity

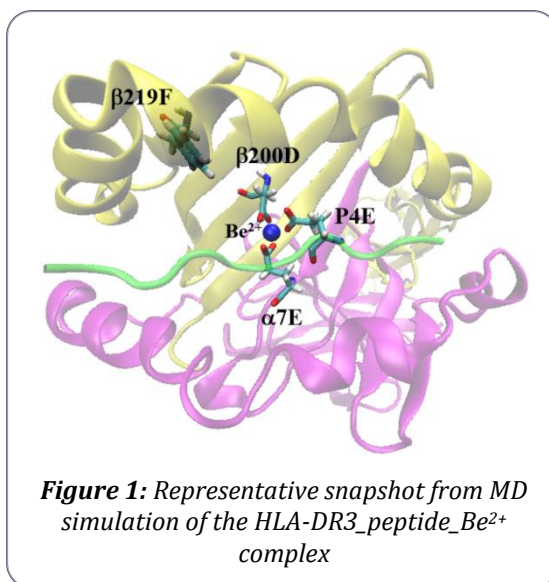
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**Keywords:** Hypersensitivity, MD simulation, Mutation.

Beryllium exposure leads to beryllium sensitization and Chronic beryllium disease (CBD) which is a granulomatous lung disease caused by accumulation of Be-responsive CD4<sup>+</sup> T-cells in the lower respiratory tract.<sup>1</sup> Beryllium hypersensitivity and CBD is mainly associated with HLA-DP alleles having glutamate residue at 69<sup>th</sup> position of  $\beta$  chain.<sup>2</sup> In HLA-DP<sub>Glu69</sub> negative individuals, HLA-DR<sub>Phe47</sub> is the susceptible marker of beryllium hypersensitivity.<sup>3</sup> However, the potential Be<sup>2+</sup> binding site on the HLA-DR allele is unknown because the natural presenting peptide is unknown. Hence, molecular dynamics (MD) simulations were carried out to identify the appropriate peptide-Be<sup>2+</sup> ion combinations that can bind to HLA-DR3 protein (Figure 1). The binding free energies calculated using MM-GBSA method suggest potential binding site of Be<sup>2+</sup> ion on modelled protein-peptide complex.



**Figure 1:** Representative snapshot from MD simulation of the HLA-DR3\_peptide\_Be<sup>2+</sup> complex

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OP 02

**Dielectric and EMI Shielding Properties of Hybrid Filler incorporated Natural Rubber Composites**

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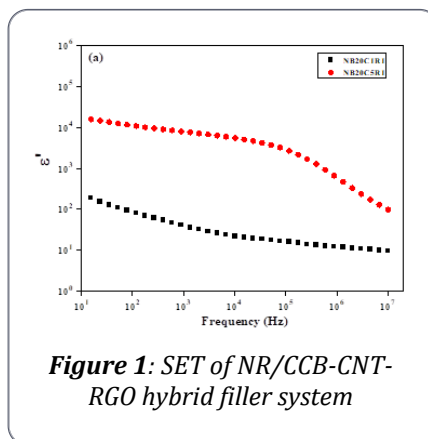
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**Keywords:** EMI shielding, Natural rubber, Hybrid filler Composites, Ionic liquid.

Conductive elastomers have significant technological promise in the current world. The work focuses on the fabrication of high-performance conductive rubber composites by integrating natural rubber(NR) with a combination of carbon-based conductive fillers and ionic liquid-modified fillers. Unlike traditional metallic conductors, these elastomers offer advantages such as easy processability, flexibility, and cost-effectiveness. Electromagnetic interference (EMI) shielding property refers to the effectiveness of a material or structure in attenuating or blocking electromagnetic radiation and preventing its interference with electronic devices or systems. The primary objective of this work is to enhance the electrical properties and EMI shielding of NR, focusing on improving interfacial interaction and dispersion of hybrid fillers within the rubber matrix.

The chosen carbon-based fillers include conductive carbon black, carbon nanotubes, and reduced graphene oxide. These properties of the composites are evaluated in terms of the homogeneous dispersion of fillers, as well as the physicochemical interfacial interactions established between the filler and the polymer matrix. EMI shielding performance of NR/hybrid filler systems is measured in the X-band frequency as it is important in modern wireless communication devices. The commercial requirement for an EMI shielding device is satisfied by all hybrid filler systems and the highest EMI SE of 33.8 dB in the frequency range of 9-10 GHz is observed for the combination of conductive carbon black, carbon nanotubes, and reduced graphene oxide. Figure 1 shows the total shielding effectiveness values in dB of NR/hybrid filler system against frequency in GHz



**Figure 1:** SET of NR/CCB-CNT-RGO hybrid filler system

## Studies on Indolo[3,2-*a*]carbazole Based Small Molecular Mass Hole-Transporting Materials for Photovoltaic Applications

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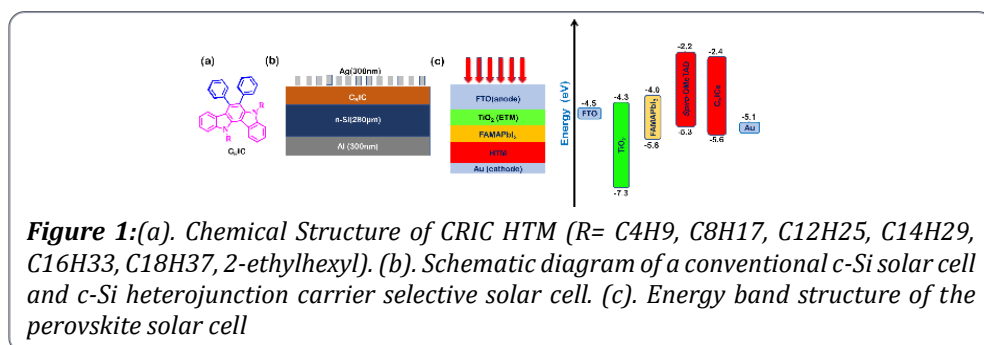
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**Keywords:** Heterocycles, Hole Transport Layer, Silicon Solar Cells, Perovskite Solar Cells.

Heterocyclic compounds possess excellent electronic characteristics, which make them suitable for organic opto-electronics.<sup>1-2</sup> The study presents the use of indolo[3,2-*a*]carbazole (CrIC) as a low molecular weight hybrid heterocycle as a hole-transporting material (HTM) in solar cell applications. The design of HTMs was based on quantum mechanical calculations (DFT) in the ground state. The CrIC structural variants were designed to enhance its solubility and hydrophobicity by altering the alkyl chain length on heterocyclic N-atom (Figure 1). The molecules were synthesized through an acid-catalyzed condensation reaction of the corresponding indole in good yield. The CrIC HTMs have excellent thermal stability, possess amorphous nature, and suitable photophysical, electrochemical, and optoelectronic properties, these all makes CrIC a good HTM candidate for perovskite and silicon solar cell applications. The CrIC possesses HOMO energy of -5.61 eV and a bandgap of 3.26 eV, which is a favorable band alignment with the valence band (VB) edge of perovskite as well as silicon absorber materials. The photovoltaic characteristics of silicon, as well as perovskite solar cells, have been thoroughly examined and achieved promising initial values. Efforts to further optimize the solar cell parameters are in progress.



**Figure 1:**(a). Chemical Structure of CRIC HTM ( $R = C_4H_9, C_8H_{17}, C_{12}H_{25}, C_{14}H_{29}, C_{16}H_{33}, C_{18}H_{37}, 2\text{-ethylhexyl}$ ). (b). Schematic diagram of a conventional *c*-Si solar cell and *c*-Si heterojunction carrier selective solar cell. (c). Energy band structure of the perovskite solar cell

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**OP 04**
**Design, Synthesis, Anti-Mycobacterial Activity, Molecular Docking and ADME Analysis Of Spiroquinoxaline-1,2,4-Oxadiazoles Via [3+2] Cycloaddition Reaction Under Ultrasound Irradiation**

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**Keywords:** Spiroquinoxaline-1,2,4-oxadiazoles, Mycobacterium tuberculosis, Cytotoxicity activity, Molecular docking, ADME properties.

The development of anti-tuberculosis (anti-TB) drugs has become a challenging task in medicinal chemistry. This is because *Mycobacterium tuberculosis* (TB), the pathogen that causes tuberculosis, has an increasing number of drug-resistant strains, and existing medication therapies are not very effective. This resistance significantly demands new anti-TB drug profiles. Here, we present the design and synthesis of a number of hybrid compounds with previously known anti-mycobacterial moieties attached to quinoxaline, quinoline, tetrazole, and 1,2,4-oxadiazole scaffolds. A convenient ultrasound methodology was employed to attain spiroquinoxaline-1,2,4-oxadiazoles via [3+2] cycloaddition of quinoxaline Schiff bases and aryl nitrile oxides at room temperature. This approach avoids standard heating and column chromatography while producing high yields and shorter reaction times. The target compounds **3a-p** were well-characterized, and their *in vitro* anti-mycobacterial activity (anti-TB) was evaluated. Among the screened compounds, **3i** displayed promising activity against the *Mycobacterium tuberculosis* cell line H37Rv, with an MIC<sub>99</sub> value of 0.78 µg/mL. However, three compounds (**3f**, **3h**, and **3o**) exhibited potent activity with MIC<sub>99</sub> values of 6.25 µg/mL. To further understand the binding interactions, the synthesized compounds were docked against the tuberculosis protein 50EQ using *in silico* molecular docking. Moreover, the most active compounds were additionally tested for their cytotoxicity against the RAW 264.7 cell line, and the cytotoxicity of compounds **3f**, **3h**, **3i**, and **3o** was 27.3, 28.9, 26.4, and 30.2 µg/mL, respectively. These results revealed that the compounds **3f**, **3h**, **3i**, and **3o** were less harmful to humans. Furthermore, the synthesized compounds were tested for ADME qualities, and the results suggest that this series is useful for producing innovative and potent anti-tubercular medicines in the future.

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## Employing Bioactive Heterocyclic Chalcones as Reaction Partners for the One-Pot Synthesis of Tetrahydro- $\beta$ -carboline based Dispiro Heterocycles

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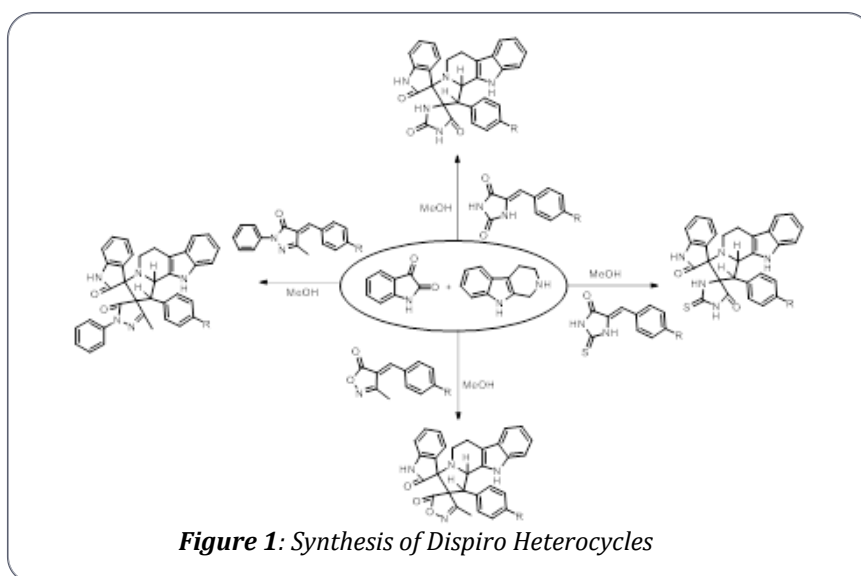
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**Keywords:** Cycloaddition, Dispiro Heterocycles, Chalcones, Azomethine ylide.

Spiro heterocycles exhibit interesting biological properties due to the presence of spirocyclic quaternary carbon stereocenter which offer an enhanced conformational rigidity to the molecule.<sup>1</sup> 1,3-Dipolar cycloaddition reaction of azomethine ylides with carbon-carbon double bonds containing electron withdrawing groups is one of the powerful synthetic approach towards the construction of many spiro compounds.<sup>2</sup> Tetrahydro- $\beta$ -carbolines (TH $\beta$ Cs) are structural motifs in many naturally occurring indole based alkaloids and can be synthesized *via* Pictet-Spengler cyclization of tryptamines.<sup>3</sup> These alkaloids exhibit remarkable biological properties including anticancer, antiviral and antioxidant activities.<sup>4</sup> The utilization of TH $\beta$ C in azomethine ylide generation with isatin has been explored for the synthesis of monospiro heterocycles using chalcones as dipolarophiles.<sup>5</sup>

The one-pot synthesis of dispiro heterocyclic compounds by the reaction of tetrahydro- $\beta$ -carboline (TH $\beta$ C) derived azomethine ylide (AY) with various bioactive heterocyclic chalcones (aldehyde adducts of pyrazolone, isoxazolone, hydantoin and thiohydantoin) are represented in Figure 1. The reactions were conducted in methanol and were found to be general with respect to isatin and chalcone. All products were isolated by column chromatography in excellent yields and were characterized by spectroscopic techniques. The synthesis and spectral characterization of the dispiro compounds will be presented.





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## Stereoselective Synthesis, *In Silico* And *In Vitro* Anticancer Evaluation And Chalcogen Interaction Study of Dispiropyrrolidine Oxindoles Obtained by the One-Pot Reaction of Isatin, Benzyl Amine and a Thiazolo[3,2-*A*]Indole Derivative

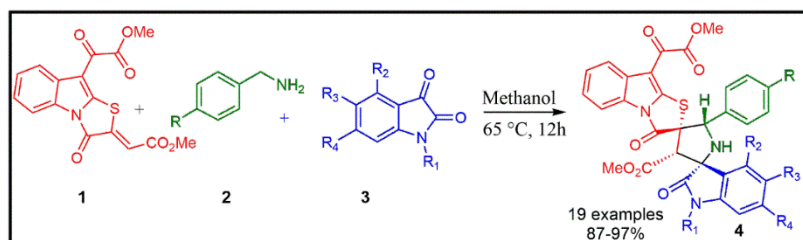
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**Keywords:** Spirooxindoles, S•••O chalcogen interaction, anticancer.

Spiroheterocycles especially spiropyrrolidines and spirooxindoles are well-known biologically promising scaffolds especially in the field of medicinal chemistry and drug discovery.<sup>1</sup> The potential of these bicyclic frameworks to act as anticancer agents, especially their active participation in MDM2-p53 pathway is noticeable.<sup>2</sup> It is well-known that conformational locking by non-covalent S•••O chalcogen interactions play a prominent role in the drug action of pharmaceutically active molecules.<sup>3</sup> Spiroheterocyclic hybrids from our group showcased potent activity against MCF-7 breast cancer cell line.<sup>5a-b</sup> In continuation of our efforts to synthesize spiroheterocycles with enhanced bioactivity, we carried out the one-pot reaction of isatin, benzyl amine and a thiazolo[3,2-*a*]indole derivative (newly synthesized in our lab)<sup>5</sup> and also did detailed investigations regarding the anticancer activity of the product by *in silico*, *in vitro* and S•••O chalcogen interaction study. A total of 19 stereoselective dispiroheterocycles of the type **4** (scheme 1) were synthesized and were fully characterized by FTIR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, CHN analysis. The structure was unambiguously confirmed by single crystal XRD analysis. Selected compounds were tested for their anticancer activity by both *in silico* and *in vitro* studies. Four single crystals of the cycloadducts were analyzed for their S•••O chalcogen bonding interactions by QTAIM and LOL plots for their role in conformational locking and affinity towards the biological target. The details of the studies done will be presented.



**Figure 1:** Synthesis of dispiropyrrolidine oxindole

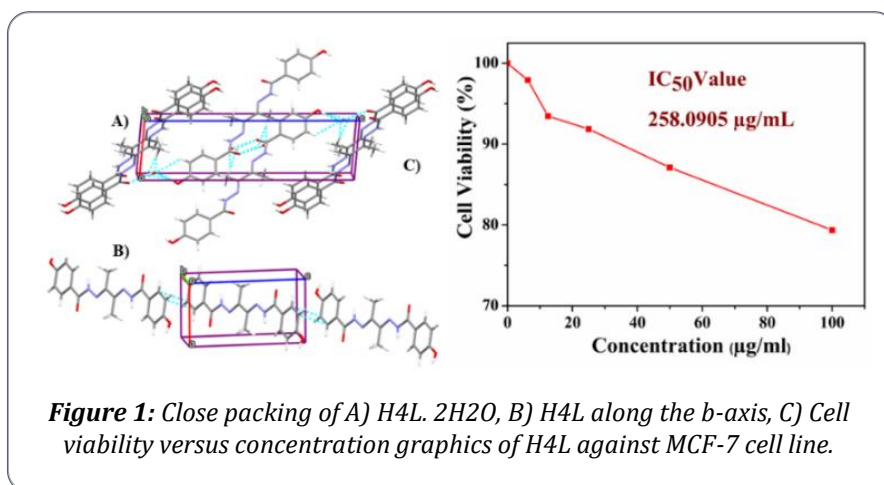
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## OP 07

**Crystal Structures, Hirshfeld Surface Analyses and DFT Study of A Novel Anticancer Proligand Butane-2,3-diylidene bis(4-hydroxybenzohydrazide)**M. Sooraj<sup>a</sup>, E. Manoj<sup>a\*</sup><sup>a</sup>Department of Applied Chemistry, Cochin University of Science and Technology, Kochi, Kerala, India. manoj@cusat.ac.in**Keywords:** Polymorphism, DFT, Hirshfeld surface analysis, Hydrazone, Anticancer

Hydrazones and their derivatives have significant anticancer activity with minimal toxicity and maximal effects and this results in the importance among researchers in cancer treatment and the development of new biologically active drug molecules.<sup>1</sup> Here we report a novel proligand butane-2,3-diylidene bis(4-hydroxybenzohydrazide) (H<sub>4</sub>L) and its characterization by different spectroscopic and analytical methods. The crystal structures of two new polymorphic forms, H<sub>4</sub>L and H<sub>4</sub>L. 2H<sub>2</sub>O, were confirmed by single-crystal X-ray diffraction. Different intermolecular hydrogen bonding interactions (Figure 1A & B) result into different lattice packing in the polymorphs. The intermolecular interactions are quantified by Hirshfeld surface analyses, which reveal that after H...H interactions, O...H interactions have a significant contribution to the total Hirshfeld surfaces in both the crystal structures. The solid-state band gap (E<sub>g</sub>) is determined experimentally as 2.57 eV using the Kubelka-Munk model. The theoretical band gap for H<sub>4</sub>L in the gas phase is, however, found to be 4.25 eV. The compound obeys Lipinski's and Veber's rules and shows drug-likeness behaviour. The *in vitro* anticancer activity of H<sub>4</sub>L against human breast cancer cells (MCF-7) is found to be promising with an IC<sub>50</sub> value of 258.1 µg/mL. (Figure 1C).



**Figure 1:** Close packing of A) H<sub>4</sub>L. 2H<sub>2</sub>O, B) H<sub>4</sub>L along the b-axis, C) Cell viability versus concentration graphics of H<sub>4</sub>L against MCF-7 cell line.

**Reference**

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## OP 09

## Synthesis, Characterization, And Metal Ion Recognition Properties Of a Triazole Linked Schiff Base Derivative of Pillar[5]Arene

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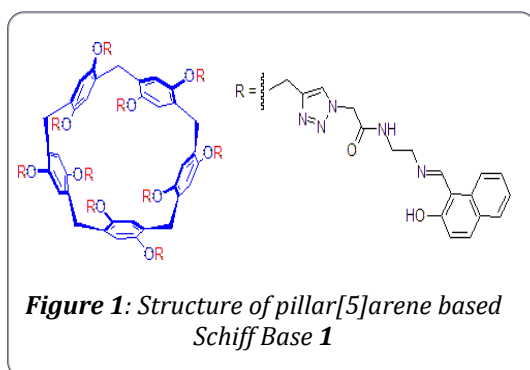
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**Keyword:** Pillar[n]arenes, host-guest chemistry, triazole, metal ions, halogens.

Metal ions are essential for many biological processes while its overload and deficiency are detrimental to life. Hence, the development of suitable receptors and methods with the highest selectivity and lowest detection limit is a challenging area of research. Although several synthetic receptors have been reported in the literature for the selective detection of ions and molecules, supramolecular-based systems offer many benefits because of their unique characteristics. Among various supramolecular systems, pillar[n]arenes have shown excellent binding affinity towards various guest molecules.<sup>1-2</sup>

In the present study, a Schiff base comprising naphthylimine linked to the pillar[5]arene platform via a triazole linker (**1**) has been developed, and investigated its binding affinities with various metal ions using spectroscopic and colorimetric techniques. Through visual colour changes, it has been found that the pillar[5]arene derivative, **1** exhibits selectivity towards Fe<sup>3+</sup> among the thirteen metal ions studied. While **1** shows

significant changes in the absorption spectra with Cu<sup>2+</sup>, Fe<sup>3+</sup>, and Al<sup>3+</sup> as demonstrated by UV-visible spectroscopy. Further, the sensor molecule, **1** is found to be selective for Al<sup>3+</sup> by *turn-on* mechanism with a fluorescence enhancement fold of ~ 34. The *in-situ* prepared Al<sup>3+</sup> complex of **1** exhibits selectivity towards F<sup>-</sup> among halogens by displacement mechanism.



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## Natural Polymer Based AWH System

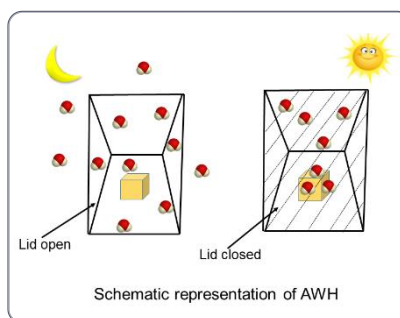
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**Keywords:** Atmospheric water harvesting, Natural polymers, Graphene oxide

The global issue of freshwater scarcity poses a significant challenge, particularly in light of population growth and worsening water pollution. Researchers are exploring the underutilized resource of atmospheric moisture, seeking solutions to address this pressing problem. A recent focus involves Atmospheric Water Harvesting (AWH) through moisture sorption using suitable sorbents.<sup>1,2</sup> This approach, combined with the efficient utilization of sunlight to release the collected water, offers



an energy-efficient and sustainable solution to address water scarcity. Hygroscopic materials and other synthetic moisture absorbing materials derived from polymers are usually adopted in moisture absorbing systems.<sup>3</sup>One significant drawback of using hygroscopic materials for moisture sorption is their leaching, and for synthetic super moisture-absorbing materials, their non-biodegradable nature. To address both these issues simultaneously, environmentally friendly moisture-harvesting materials, like natural polymers are being explored. These materials exhibit moisture sorption properties, and can trap moisture from atmosphere. Furthermore, with the assistance of materials like Graphene oxide that possesses photo thermal conversion efficiency, release of absorbed moisture can be effectively facilitated. In this context, we present a novel approach involving the incorporation of graphene oxide into neem gum polymer for efficient atmospheric water harvesting. The material can absorb approximately 1.8g/g of water within a short period of 2 hours and about 3.29g/g of water over 24 hours at a relative humidity of 75% at 28°C. Additionally, it demonstrates approximately 10 times reusability, offering a promising solution to the challenges of water scarcity. Other advantageous characteristics including low cost, ease of scaling up, and portability make it a promising candidate for commercialization, offering a potential solution to the critical issue of freshwater scarcity.

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## OP 11

### Picric Acid Detection Using Luminescent Carbon Nanoparticles

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**Key words:** Nitroaromatic compounds, carbon nanodots, luminescence

Nitroaromatic compounds (NACs) constitute a class of industrially significant species which find various applications. Unfortunately, the widespread use of NACs causes serious environmental contamination concerns<sup>1</sup>. The current approaches to detect and remove NAC from the environment are frequently insufficient and unsustainable, which leads to their unintentional release into the environment. Therefore, developing a convenient and reliable platform for its fast and efficient detection is of paramount importance from security point of view. Among the NACs, picric acid (2,4,6-trinitrophenol) is more harmful to the environment and has caused much worry in society. Here we have synthesized orange-red fluorescent carbon nanodots (PD-CDs) for the selective, sensitive and rapid determination of picric acid<sup>2</sup>. PD-CDs are well characterized using High Resolution Transmission Electronic Microscopy (HR-TEM), X-Ray Diffraction (XRD) Analysis, Fourier Transform Infra-Red (FT-IR) Spectroscopy, X-Ray Photoelectron Spectroscopy (XPS), UV-Visible Absorbance spectroscopy, Raman spectroscopy and Fluorescence spectroscopy. Luminescence quenching in carbon nanodots<sup>3</sup> upon the addition of picric acid paves the way to fluorimetric detection of picric acid at micromolar concentrations, with limit of detection 17.23  $\mu\text{M}$ . Additionally, a mechanism is proposed for picric acid induced luminescence quenching in carbon nanodots.

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# POSTER PRESENTATIONS

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## Crystal Structures, DFT and Photocatalytic Studies of Two Novel Thiosemicarbazone Based Proligands

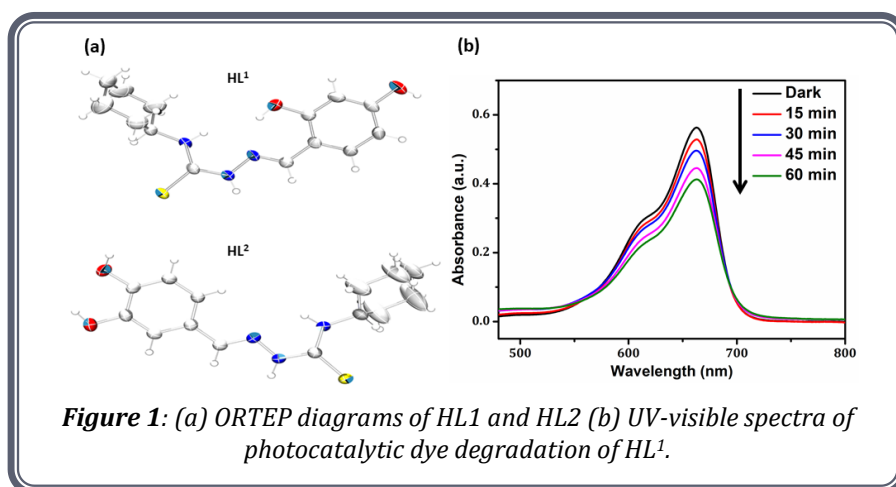
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**Keywords:** Thiosemicarbazone, SCXRD, Hirshfeld, DFT, Photocatalysis

Thiosemicarbazones receive continuous scientific attention due to their interesting characteristics in industrial applications<sup>1</sup>. Two novel Schiff base ligands 2,4-dihydroxybenzaldehyde-N(4)-cyclohexylthiosemicarbazone [HL<sup>1</sup>], and 3,4-dihydroxybenzaldehyde-N(4)-cyclohexylthiosemicarbazone [HL<sup>2</sup>] were synthesized and characterized by CHNS, IR, UV-vis and UV-DRS. The structures were then confirmed by X-ray crystallography. The relevant intermolecular interactions of both the ligands were quantified using Hirshfeld surface (HS) analyses. The ligands exhibit stronger isotropic H...H interaction contribution (55.1 % For HL<sup>1</sup> and 54.4% for HL<sup>2</sup>) to the overall HS, indicating that the van der Waals forces are the dominating factor and are seen in the middle of the scattered point of the 2D fingerprint plots. The geometrical optimization and theoretical calculations of the compounds were achieved by DFT using B3LYP/6-311G (d,p) basis sets. The direct bandgaps of the compounds were calculated experimentally using the Kubelka-Munk model, which shows 2.19 eV for HL<sup>1</sup> and 3.05 eV for HL<sup>2</sup>. The photocatalytic activities of the proligands HL<sup>1</sup> and HL<sup>2</sup> were examined for the degradation of methylene blue under visible light irradiation, which is found useful and the prospective metal complexes would be promising candidates for photocatalytic activities.



**Figure 1:** (a) ORTEP diagrams of HL1 and HL2 (b) UV-visible spectra of photocatalytic dye degradation of HL<sup>1</sup>.

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## PP 02

**Optimization of Porphyrin – Monomers as Building Units of Polymer Molecular Photoelectrodes for Solar Fuel Generation**Aparna C.<sup>a</sup>, Arifa K. V. <sup>a</sup>, Haritha A. P. <sup>a</sup>, Fazalurahman K.<sup>a\*</sup><sup>a</sup>*Solar and Electrochemical Energy Lab, Department of Chemistry, University of Calicut, Malappuram, Kerala, India.*

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In response to the global energy demands of the growing population, it becomes imperative to generate an environmentally sustainable source of energy. The enormous utilization of fossil fuels as the feedstock to meet the current global demand releases a massive amount of atmospheric CO<sub>2</sub>. The increase in the concentration of atmospheric CO<sub>2</sub> leads to global warming and related climate changes. Technologies for direct capturing and conversion of greenhouse gaseous like CO<sub>2</sub> will lead to lower the atmospheric CO<sub>2</sub> level and thus furnish a solution for environmental concerns like global warming. Functional bio-inspired molecular catalysis provides a clear idea on the mechanistic aspects, tunability, metal atom economy and high-selectivity for catalytic cycles compared to the heterogeneous semiconductor photocatalysts<sup>1</sup>. Porphyrin-based redox photosensitizers (PS) or catalyst units (CAT) have got significant attention for their application in various processes of solar fuel generation. Efficient strategies for immobilizing molecular building units on semiconductor lattice is the key-step for the fabrication of molecular photo-electrodes. However, the lower loading density, and poor adsorption stability of the porphyrin molecules on semiconductor lattice limits practical feasibility of molecular photoelectrodes. Herein, We synthesized two porphyrin derivatives which are 5,10,15,20-tetrakis(α pyrrol-p-tolyl) porphyrin (PyrPor) and tetrastyrilporphyrin (Vinylpor). The active functional groups were incorporated which are pyrrole and vinyl for oxidative and reductive polymerization respectively. An in situ electropolymerizing strategy were used for immobilizing the porphyrin molecules on the surface of rutile TiO<sub>2</sub> semiconductor lattice. The photoelectrochemical studies were performed by using polymerized electrode on FTO as the working electrode, with Ag/AgCl as the reference and Pt- as the counter electrode. The photo response of the electrode upon visible light irradiation indicates the electron injection from the excited porphyrin molecules on the surface into the conduction band of TiO<sub>2</sub> particles.

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## Main-group Organometallic Compounds for Versatile Applications

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**Keywords:** Triarylboranes, Photophysics, D-A conjugates, Fluoride sensors.

Air stable main group organometallic compounds (M.O.C) gained much interest in the recent years due to impressive photophysical properties attributed to their inherently electron deficient nature and their ability to extend conjugation.<sup>1</sup> The unique photochemistry of M.O.C were successfully exploited in the development of NLOs, TPA (two photon absorption) as well as colour tunable emissive materials for OLEDs.<sup>1</sup> Apart from these, the Lewis acidic M.O.C centre can also accommodate small anionic Lewis bases (F<sup>-</sup>, CN<sup>-</sup>) via covalently bound adduct formation, allowing their usage as reversible receptor sites for such species which makes it potential fluorescent and chromogenic anion-sensors.<sup>2</sup> Our research primarily focuses on designing of single colour solid state emitting materials for the OLED applications and, therefore, as our pioneer work, we have reported three main group organometallic triarylborane-triphenylamine based donor-acceptor conjugates with solid state emitting properties, in the year 2022.<sup>3</sup> Our designed star shaped triarylborane-triphenyl amine D-A system were fine-tuned via introduction of additional donor/acceptor moiety, creating A-D-DD and A-D-AA type molecules and their optical characteristics were evaluated. Additionally, we are highlighting two TPA-TAB D-A conjugates, functionalized by dimethylamino moiety, which can show excellent pH sensing ability. All the five TAB-TPA D-A conjugates showed typical intramolecular charge transfer luminescence with solvatochromic fluorescence emission. Moreover, our compounds 1,4-5 shows a *turn-on* response towards fluoride ion with a detection limit of 0.38-0.39  $\mu\text{M}$  range, as well as to acidic pH condition, which draws wide focus towards the analytical field.

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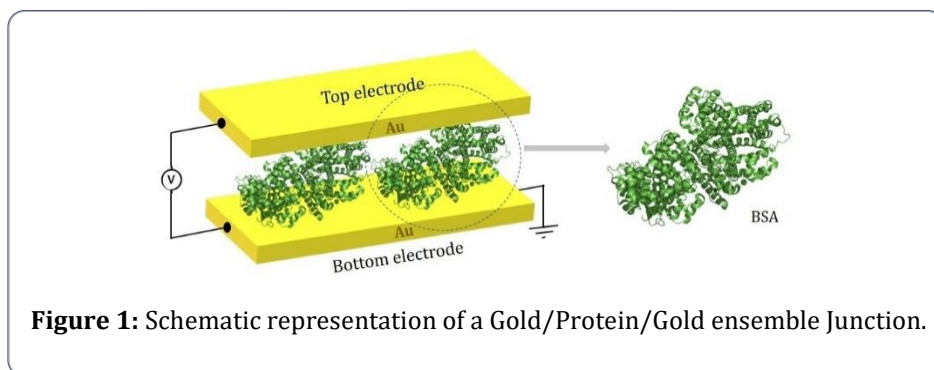
## PP 04

**Understanding the Mechanism of Charge Transport via Non-Redox Active Proteins in Solid-State Configuration**Aswany Gopal<sup>a</sup>, Jerry A. Fereiro<sup>a\*</sup>*School of Chemistry, Indian Institute of Science Education and Research Trivandrum (IISER TVM), Vithura, Kerala, India.*

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**Keywords:** Biomolecular electronics, charge transport, non-redox proteins

A family of proteins called redox-active proteins are known to play vital roles in the charge transport pathways in many biological processes, such as respiration and photosynthesis. Therefore, these proteins have been actively studied<sup>[1-3]</sup> in the field of biomolecular electronics.<sup>[4]</sup> Interestingly, some non-redox active proteins have also been demonstrated with similar charge transport behavior.<sup>[5]</sup> Previous studies have reported their electron transport properties in the solvent phase, but their electron transport (ETp) characteristics in solid states remain largely unexplored. Currently, we are investigating the ETp properties of such a non-redox active protein called bovine serum albumin (BSA) in the solid state. In this study, we investigate the modulation of BSA's band gap by doping with different metal derivatives of an organic molecule called tetraphenyl porphyrin (TPP). The primary aim of our project is to tune the energy levels of proteins by doping different metal centers on TPP and thereby control the charge transport mechanism via protein junctions (Figure 1). The outcomes of this study will significantly aid in the development of biomolecular devices such as transistors, switches, and diodes.

**Figure 1:** Schematic representation of a Gold/Protein/Gold ensemble Junction.**References**

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## **Polyaniline/Carbon Sphere-Graphene Ternary Nanocomposite Material for Asymmetric Supercapacitors**

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**Keywords:** Polyaniline/carbon sphere-graphene; In-situ polymerization; High performance supercapacitor

High power density, long cycle life, and fast charge-discharge rates make supercapacitors promising candidates for energy storage.<sup>1</sup> Although polyaniline has a high theoretical capacitance, its use as a supercapacitor electrode material is limited due to its low cycling efficiency.<sup>2,3</sup> In the present work, a ternary nanocomposite is prepared by combining polyaniline (PANI) with carbon sphere and graphene. The synergetic effect of the materials eliminates their drawbacks when used individually. Here, PANI inhibits graphite layer restacking, whereas carbon sphere-graphene eliminates PANI agglomeration. Strong interaction between PANI and carbon sphere-graphene is also proved from material characterization studies. An asymmetric coin cell having high cyclic stability and power density is also fabricated using the ternary nanocomposite demonstrating the suitability of the electrode in real sense energy storage applications.

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**PP 06**
**Comparative Study of the Photocatalytic Activity Of g-C<sub>3</sub>N<sub>4</sub>/Mn<sub>4</sub> (M=Mn, Fe, Co) for Water Splitting Reaction**

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**Keywords:** DFT, Photocatalyst, Modelling

In this study, novel nanocomposites of g-C<sub>3</sub>N<sub>4</sub>/MN<sub>4</sub> (where M is Mn, Fe, or Co) were designed using advanced density functional theory (DFT). The cutting-edge DFT method was employed to evaluate the photocatalytic activity of the g-C<sub>3</sub>N<sub>4</sub>/MN<sub>4</sub> (M=Mn, Fe, and Co) composites. A comprehensive analysis was conducted on the geometry, electronic, optical properties, work function, charge transfer interaction, and adhesion energy of the g-C<sub>3</sub>N<sub>4</sub>/MN<sub>4</sub> (M=Mn, Fe, and Co) heterostructure. Lastly, the potential of the g-C<sub>3</sub>N<sub>4</sub>/MN<sub>4</sub> (M=Mn, Fe, and Co) heterojunction as a photocatalyst for the water splitting reaction was assessed by examining its band alignment for the water splitting reaction. Ideally, for water splitting, the valence band maximum (VBM) band position should be higher than the O<sub>2</sub>/H<sub>2</sub>O potential (0 V vs. NHE), and the conduction band minimum (CBM) band position should be lower than the H<sup>+</sup>/H<sub>2</sub> potential (1.23 V vs NHE). The g-C<sub>3</sub>N<sub>4</sub>/FeN<sub>4</sub> and g-C<sub>3</sub>N<sub>4</sub>/CoN<sub>4</sub> composites meet this requirement, making them suitable for use as photocatalysts for water splitting.

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## Synergistic g-C<sub>3</sub>N<sub>4</sub>/Graphene Hybrid Nanocomposite Electrode Material with Ultrahigh Specific Capacitance

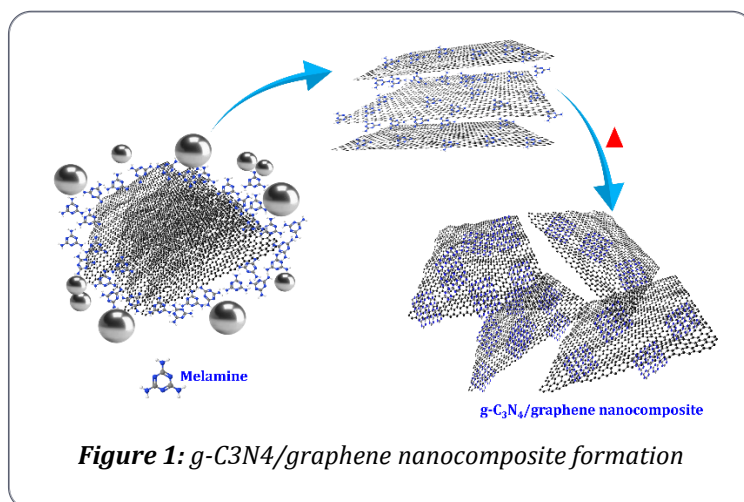
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**Keywords:** Graphene, g-C<sub>3</sub>N<sub>4</sub>, Supercapacitor

The bulk polymeric structure of g-C<sub>3</sub>N<sub>4</sub> and multilayer structured graphite is less conducting in nature than their 2D counterparts, which limits their electrochemical applications. Here a combination of the 2D materials g-C<sub>3</sub>N<sub>4</sub> and graphene through synchronous top-down and bottom-up pathways is employed to prepare g-C<sub>3</sub>N<sub>4</sub>/graphene hybrid nanocomposite (Figure 1). Their synergistic combination exhibited an ultrahigh specific capacitance which is having 100% retention even after many continuous charge-discharge cycles. Mechanochemical graphite exfoliation offers graphene with reduced defects and rich nitrogen doping to contribute towards specific capacitance and better energy density. The prepared material was characterized by XRD, FTIR spectroscopy, FESEM, Raman spectrum, and HRTEM. The charge-discharge curves exhibit a minor pseudocapacitance nature which is in agreement with results from the Dunn's method. Nyquist plot of the nanocomposite shows lower charge transfer resistance.



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**PP 08**
**Nitrogen-Doped Nickel Mofs as Efficient Electrode Material for Supercapacitor Applications**

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**Keywords:** Metal organic frameworks, supercapacitors, galvanostatic charge/discharge, cyclic voltammetry

Metal organic frameworks are most favorable material for supercapacitor applications. We followed a polyvinylpyrrolidone (PVP) assisted strategy for the preparation of Nitrogen doped Ni MOF (N-Ni MOF). Here, PVP acts as both a nitrogen source and structure-directing reagent. N-Ni MOF was synthesized through solvothermal method using PVP. The effect of PVP on the morphology and electrochemical performance of Ni MOF electrodes for supercapacitors was investigated in detail. The structural features of the designed material were characterized using X-ray diffraction, Fourier transform infrared spectroscopy, Scanning electron microscopy, Transmission electron microscopy, Brunauer-Emmett-Teller (BET) method, and X-ray photoelectron spectroscopy. Cyclic voltammetry and galvanostatic charge-discharge tests were used to assess the supercapacitive characteristics. The nitrogen-doped Ni MOF appeared hierarchical flower-like microsphere morphology with a high surface area compared to Ni MOF. Moreover, N-Ni MOF exhibited superior performance with a high specific capacitance of 1519F/g at a current density of 1A/g. An all-solid-state symmetric supercapacitor assembled using N-Ni MOF as an electrode and PVA/ KOH gel as an electrolyte delivered a specific capacitance of 529F/g at 0.5 A/g. This device exhibits a significant energy density of 66.12WhKg<sup>-1</sup> with a power density of 900.3Wkg<sup>-1</sup> and also retains stability of 89 % even after 2000 cycles at a current density of 1A/g.

## **A Comparative Study on the Effect of Protic and Aprotic Ionic Liquid Doping in Polyaniline**

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Polyaniline is a conducting polymer with immense applications including energy storage devices like supercapacitor. The properties of polyaniline greatly depend on the dopant ion present. The dopant ion is responsible for creation of charge carriers in the polymer chain and thus allowing the polymer to conduct electricity. In our present work we studied the effect of ionic liquids in the properties of polyaniline. We initially synthesised polyaniline with dopant as protic and aprotic ionic liquid and then the properties were compared with polyaniline synthesised with H<sub>2</sub>SO<sub>4</sub> as the dopant. The FTIR spectrum suggests that the structure of polyaniline is similar to that of polyaniline synthesised from H<sub>2</sub>SO<sub>4</sub>. It is observed that the thermal stability of the polyaniline doped with the ionic liquids is improved. There is no significant improvement in capacitance is observed when doped with the ionic liquids but the capacitive retention is greatly improved when doped with protic ionic liquid. The results point out that the doping of polyaniline with protic ionic liquids is a simple and efficient method to improve the properties.



## PP 10

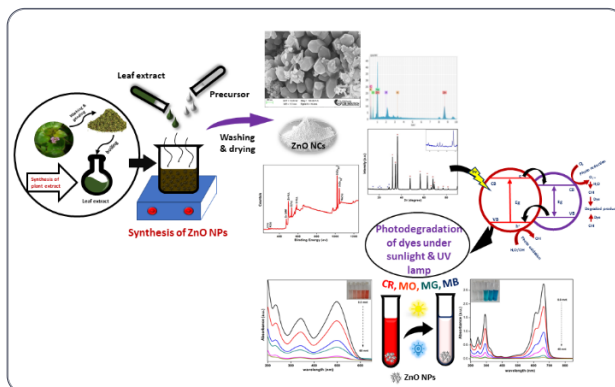
## Photocatalysed Dye Degradation Using Biogenic Zinc Nanocomposites

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**Keywords:** Metal Oxide Nanoparticles, Photocatalysis, Biogenic, Dye Degradation, Water Treatment

Biogenic zinc oxide nanocomposites (NC) were synthesized using an eco-friendly method employing *Boerhaavia diffusa* leaf extract and characterized using UV-DRS, FTIR, XPS, XRD, SAED, FESEM, EDAX, HRTEM, ICP-MS, XRF methods, and zeta potential analyses. The hexagonal wurtzite structure in ZnO alongside rod-like structures



associated with sodium and potassium agglomerates is confirmed by XRD results. This nanocomposite showed excellent catalytic activity and degrading Methylene blue and Congo red dyes in aqueous solutions under sunlight and UV illumination within specific time frames. Both cases, a catalyst quantity of 50 mg successfully removed both dyes within 40-60 minutes in sunlight and 15-30 minutes under UV illumination. It is also noted that the nanocomposites exhibited better efficacy under UV light due to their favourable semiconductor band gap of 3.26 eV. This environmentally benign approach provided a cost-effective method for producing ZnO NC suitable for photocatalytic use. The presence of potassium and sodium exhibited a synergistic effect with ZnO NC, enhancing its photocatalytic activity. The streamlined method of synthesis using sustainable and eco-friendly practice got significant attraction even though the flexible elemental composition of the composite poses a limitation due to the lack of specific precursor content. Pure zinc nitrate was the sole precursor employed for the synthesis apart from the extract, resulting in the zinc nanocomposite containing notable concentrations of potassium, phosphorus, sodium, zinc, and oxygen. Remarkably, the consistent elemental ratio was achieved through this green synthetic route, utilizing elements present in the *Boerhaavia diffusa* leaf extract. This approach showcases a natural source for this refined semiconductor composite without the need for additional chemicals or routes. The composite's metal-rich nature holds promise for eliminating various organic pollutants, including pesticides and endocrine-disrupting compounds, opening doors for further investigation and applications.

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## Oxidative Amidation of Hydrazone with Carboxylic acid Under Metal-free Condition

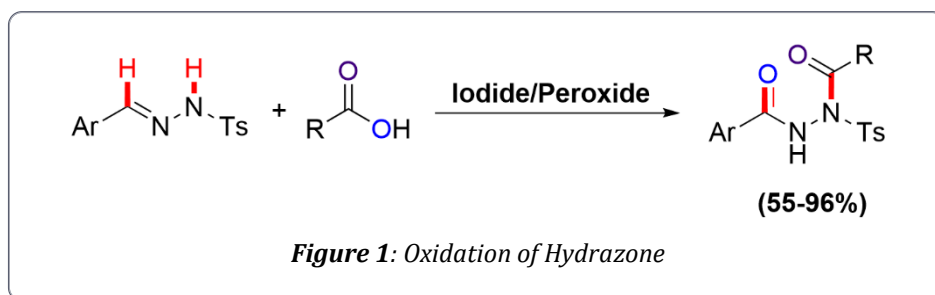
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**Keywords:** Amidation, Iodine Catalysis, Metal Free, Tosyl Hydrazones, Indazolone

Oxidative coupling reactions are quite significant in organic transformations as they enable a new carbon-carbon or carbon-heteroatom bond formation at the expense of two C-H bonds or one C-H and X-H bond each (X = O, N, S etc).<sup>1,2</sup> As the demand for green synthetic routes is increasing, metal-free approaches for oxidative coupling has attained much attention recently. Iodine catalysis have contributed significantly in this direction.<sup>3,4</sup> Here, we report an oxidative amidation of tosyl hydrazones to bisamides by treating with carboxylic acids in presence of Iodide as the catalyst and peroxide as the oxidant at room temperature. Aromatic and aliphatic acids readily afforded the amide with hydrazones of different electronic nature (Scheme 1). Further, properly functionalized bisamides were engaged in an intramolecular N-arylation reaction to afford indazolone.



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## PP 12

**Highly Active Unsymmetrical Ru(II)-NHC Complexes For Catalytical Transfer Hydrogenation Reactions; Impact Of Proximal Trifluoromethyl Group And Effective N-Coordination**Anjitha Jayaraj<sup>a</sup>, Chinna Ayya Swamy P<sup>a\*</sup><sup>a</sup>Main-group Organometallic Optoelectronic Materials and Catalysis Lab, Department of Chemistry, National Institute of Technology, Calicut, India, 673601.

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**Keywords:** N-Heterocyclic Carbene (NHC), Transfer Hydrogenation, Catalyst loading, Ru-NHC complexes

N-Heterocyclic carbene (NHC) has evolved over the last couple of decades as important class of ligand in designing versatile metal based homogenous catalyst.<sup>1</sup> The facile synthesis which allows for easy functionalization to fine-tune their stereoelectronic properties, stamped them as privileged or highly accessible ligands in the field of catalysis. On introducing chelation via tailoring the coordination geometry with bi or multidentate ligands can impart stability to catalytically active systems, and shows better performance at a low catalyst loading. Moreover, incorporating an ancillary functionalisations on NHC that influences the steric and electronic profile of metal center is preferred, so that their catalytic activity can be tweaked.<sup>2</sup>

In light of these facts, here we synthesized six differently functionalized Ruthenium(II)-NHC complexes following transmetallation route, primarily focusing to develop a low catalyst loading activity. A superior catalytic efficiency in transfer hydrogenation (TH) was demonstrated with one of the complex **Ru-1** at a low loading of 0.01 mol% for acetophenone (12 h) and 0.001 mol% for all aromatic aldehydes within 1 h. In addition, **Ru-1** outperforms the literature in becoming superior catalyst in aldehydic reduction, with a TOF of 10,000 h<sup>-1</sup>. This unexceptional catalytic activity can be attributed to the effective coordination as well as the proximal interaction of the ancillary substitute-CF<sub>3</sub> group with metal center, which in turn reduces activation energy initiating the catalytical cycle. These conversions possible at low catalyst loading for ketones and the complete conversion of all aldehydes regardless of the substituents are interesting results from the catalysis perspective.

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## Synthesis of Thiazolidinone based Pyrrolidinobisspiroindoles Through [3+2] Cycloaddition Reaction

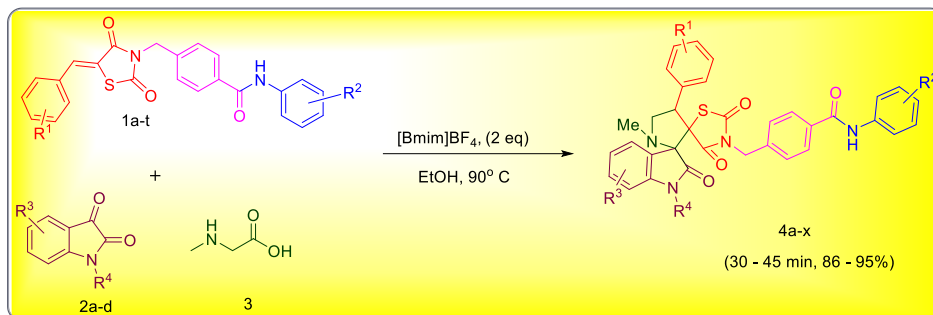
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**Keywords:** Pyrrolidino-bisspiroindoles, Ionic liquid, Thiazolidine-2,4-dione

The development of new molecules from known structural motifs through molecular hybridization is one of the trends in drug discovery. We have designed and synthesized thiazolidinone based pyrrolidino-bisspiroindoles. The targeted compounds were synthesized from thiazolidinone based chalcones (**1a-t**), with azomethine ylide generated in situ by the reaction of isatin (**2a-d**) and sarcosine (**3**). A wide variety of substrates were explored to obtain good yields (up to 95%). Thiazolidine-2,4-diones are an insulin sensitizing drug class that includes ciglitazone, pioglitazone, and rosiglitazone. Aside from their known anti-diabetic activity. Thiazolidine-2,4-dione has been shown in numerous *in vitro* and *in vivo* studies to have antibacterial, antifungal and anti-cancer activity. The target compounds thiazolidinone based pyrrolidino-bisspiroindoles (**4a-x**) were synthesized and characterized by IR, NMR, HRMS, and X-ray analysis. *In vitro* anti-cancer studies of targeted compounds (**4a-x**) are under progress.



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PP 14

**An Ultrasound Assisted Green Protocol for the Synthesis of Quinoxaline based Bisspirooxindoles: Crystal Structure Analysis, Enone Umpolung, DFT Calculations, Anti-Cancer Activity and Molecular Docking Studies**

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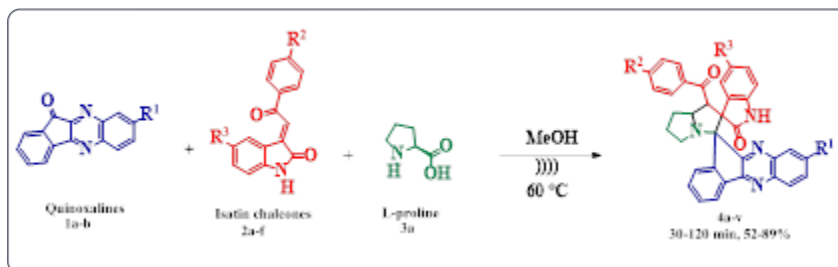
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**Keywords:** Bisspirooxindoles, Ultrasonication, DFT calculations, Hirshfeld surface, Anti-cancer activity

A series of novel quinoxaline based bisspirooxindolo- pyrrolizidines were synthesized through 1,3-dipolar cycloaddition under ultrasonication with shorter reaction time and good yields. The compounds were well characterized by various spectroscopic methods and finally single crystal X-ray diffraction method (**4c**, **4d**). DFT energy calculations confirm the regioselectivity due to enone umpolung effect. The *in vitro* anti-cancer activity of the synthesized compounds (**4a-v**) shows that the compounds **4g** and **4q** exhibited good anti-cancer activity with IC<sub>50</sub> values 14.51±1.1 μM and 11.36±0.23 μM against DU-145 prostate cancer cell line; and 16.78±0.95 μM and 14.28±0.64 μM against Hela cervical cancer cell lines when compared to the standard anti-cancer drug doxorubicin (1.75±0.06 μM and 1.35±0.09 μM). *In silico* molecular docking studies indicated that the synthesized compounds may serve as potential lead for the further development of novel anti-cancer agents.



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## Rapid Detection of Ag(I) via Size-induced Photoluminescence Quenching of Biocompatible Green-Emitting, L-Tryptophan-Scaffolded Copper Nanoclusters

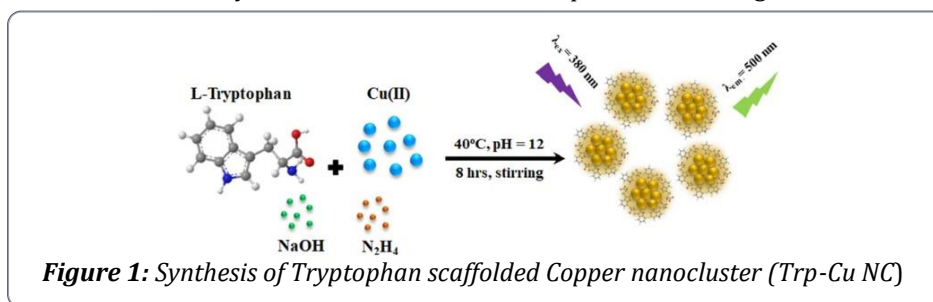
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**Keywords:** Nanocluster; Photoluminescence; Quenching; Cell-imaging; Fluorescence Resonance Energy Transfer

In this article we have reported the synthesis of a green-emitting ( $\lambda_{\text{ex}} = 380$  nm,  $\lambda_{\text{em}} = 500$  nm), single amino-acid (L-tryptophan)-scaffolded copper nanocluster (Trp-Cu NC) via a one-pot route under mild reaction conditions (Scheme 1). The synthesized nanocluster can be used for the rapid detection of a heavy metal, silver (Ag(I)), in the nanomolar concentration range in real environmental and biological samples. The strong green photoluminescence intensity of the nanocluster quenched significantly upon the addition of Ag(I) due to the formation of bigger nanoparticles. A notable colour change from light yellow to reddish-brown can also be observed in the presence of Ag(I), allowing its visual colorimetric detection. Portable paper strips fabricated with the Trp-Cu NC can be reliably used for the on-site visual detection of Ag(I) in the micromolar concentration range. The Trp-Cu NC possesses excellent biocompatibility, making it suitable nanoprobe for cell imaging; thus, it can act as an *in vivo* biomarker. The nanocluster showed significant spectral overlap with anticancer drug doxorubicin and thus can be used as an effective fluorescence resonance energy transfer (FRET) pair.<sup>1</sup> FRET results can reveal important information regarding the attachment of the drug to the nanocluster and hence its role as a potential drug carrier for targeted drug delivery within the human body.<sup>1</sup> The further details will be presented during the conference.



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## PP 16

**Citric Acid Derived Carbon Dots for Antibacterial Applications**Amrutha T. P.<sup>a</sup>, Renuka N. K.<sup>a\*</sup>*Advanced Materials Research Centre, Department of Chemistry, University of Calicut, Kerala, India.**\*renuka@uoc.ac.in***Keywords:** Carbon dots, antibacterial study, inhibition zone test

Bacterial infections pose a significant threat to human health. Excessive reliance on conventional antibiotics and antibacterial agents can lead to the proliferation of resistant bacteria. Hence, the development of novel antibacterial materials is highly demanded<sup>1</sup>. The non-toxic properties and intrinsic antibacterial efficacy of Carbon dots (CDs) have gained considerable interest in recent years. The light-induced antibacterial effect of CDs is a secure procedure with negligible side effects<sup>2</sup>. In the present work citric acid derived carbon dot has been synthesised in a one-step hydrothermal method. The system is characterized using Transmission Electron Microscope (TEM) analysis, X-Ray Diffraction (XRD) analysis, Fourier Transform Infrared (FT-IR) spectroscopy, UV-VIS Spectroscopy (UV-Vis). The antibacterial activity of CDs against Gram-negative E. coli bacteria was investigated by the inhibition zone test<sup>1, 3, 4</sup>. The diameter of inhibition zone of CDs towards E. coli bacteria was around 12mm. The direct engagement of CDs with bacterial cells adds to the overall antibacterial efficacy. The distinctive and intricate mechanisms underlying the antibacterial activity of CDs encompass the generation of reactive oxygen species (ROS), breakdown of cell structure, and cytoplasm leakage due to DNA binding and the modulation of gene expression<sup>2</sup>.

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## Lysozyme Capped Copper Nanocluster: A Tunable Dual-Metal Sensor for the Selective and Sensitive Detection of $\text{Ag}^+$ and $\text{Fe}^{2+}$

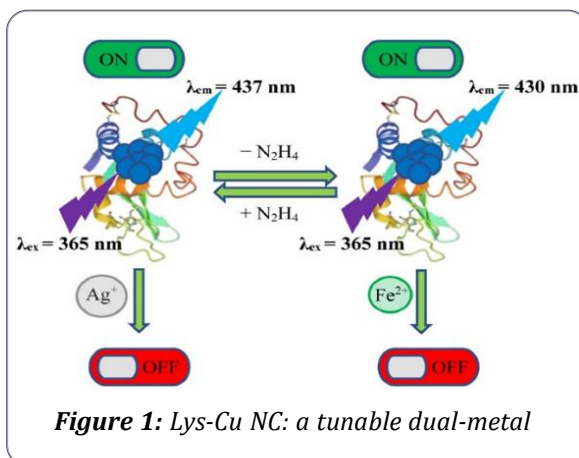
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**Keywords:** Nanocluster, Photoluminescence, Dual-metal sensor, Reducing agent, Collisional quenching

Protein protected metal nanoclusters emerged as a promising class of nano-materials due to their various interdisciplinary applications, namely as efficient metal sensors. Depending on its practical applications, the photoluminescence properties of these nanoclusters can be tuned easily. Here we have successfully designed a photoluminescent protein (lysozyme) scaffolded copper nanocluster (Lys-Cu NC) ( $\lambda_{\text{ex}} = 365 \text{ nm}$ ,  $\lambda_{\text{em}} = 437 \text{ nm}$ ) that can be used as a dual metal



sensor for the sensitive and selective detection of silver ( $\text{Ag}^+$ ) and ferrous ( $\text{Fe}^{2+}$ ) ions through two independent photoluminescence turn off mechanisms. The nanocluster when synthesized in the presence of a mild reducing agent hydrazine ( $\text{N}_2\text{H}_4$ ) can selectively detect  $\text{Ag}^+$  (LOD = 4 nM) through a size induced photoluminescence quenching method involving both static and dynamic mechanism.<sup>1</sup> The selectivity of the nanocluster can be switched back and forth between  $\text{Ag}^+$  and  $\text{Fe}^{2+}$  by simply controlling the redox properties of the medium. By removing the excess  $\text{N}_2\text{H}_4$  from the medium, the selectivity can be tuned towards  $\text{Fe}^{2+}$ , which can quench the photoluminescence intensity through a static charge transfer process.<sup>2</sup> However, the selectivity towards  $\text{Ag}^+$  can be recovered by externally adding mild reducing agent to the medium (Figure 1). Thus in this report we showed a simple method to design a dual-metal sensor which can be extended to design multi-metal sensors for a wide range of applications.

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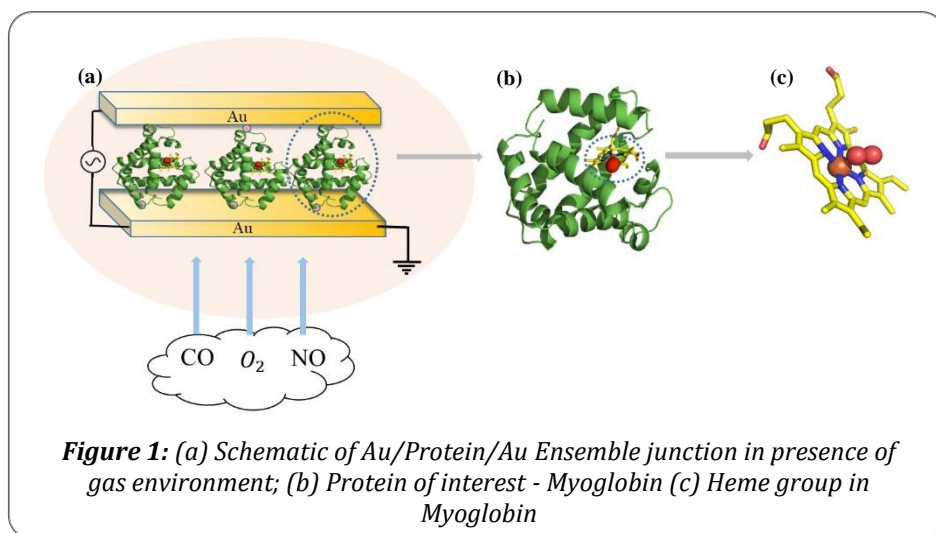
## PP 18

**The Feasibility of Using Proteins in Solid- State as Electronic Gas Sensors**Aswin S<sup>a</sup>, Jerry A. Fereiro<sup>a\*</sup><sup>a</sup>School of Chemistry, Indian Institute of Science Education and Research Trivandrum (IISER TVM), Vithura, Kerala, India.

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**Keywords:** Solid-state proteins, Charge transport, Gas Binding, Protein sensors

In nature, most interactions of proteins with each other or with other molecules or with ions occur in a solution (apart from those in membrane environments)<sup>1</sup>; *designing experiments for dry protein devices in which the protein conditions can be changed presents a formidable challenge<sup>2</sup>, one that we intend to meet in this work.* Here, we will measure ETp via Mb while exposing Mb to different types of gas molecules (see fig 1). In addition, the involvement of the Heme site in the ETp path will be measured by using Myoglobin derivatives (Apo Mb and Fe free Mb) as well as the importance of the Heme coupling to the surface by electrically wiring the Protein to the surface<sup>3</sup>. The differences measured by the real-time monitoring of the ETp before and after interacting with the Heme prosthetic group with the gas molecules will give us information about the strength of the binding of gas molecules with the Heme prosthetic group and how it influences the alignment of the frontier orbitals with respect to the  $E_F$  of the system<sup>4</sup>.



**Figure 1:** (a) Schematic of Au/Protein/Au Ensemble junction in presence of gas environment; (b) Protein of interest - Myoglobin (c) Heme group in Myoglobin

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## Synthesis of $\beta$ -Aryldinaphthoporphycenes – New Porphycene Ligands

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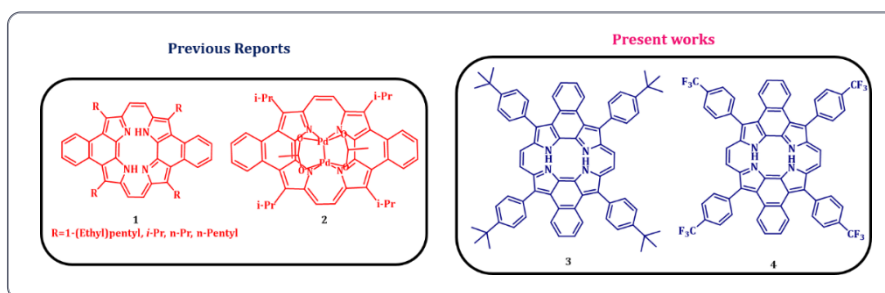
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**Keywords:** Naphthobipyrrole, Porphyrin, Dinaphthoporphycene

Naphthobipyrrole is a potentially useful building block for porphyrin and porphyrin analogue synthesis. A simple, generalizable synthetic route to  $\alpha$ -formylated,  $\beta$ -substituted naphthobipyrroles and their use in the preparation of dinaphthoporphycenes were explored independently by Sessler and Panda groups.<sup>1,2</sup> Substituents play a major role in modulating the core size of porphycene resulting in varying degree of NH...N hydrogen bonding interaction, thus affecting the coordination ability. In 2015, Panda group reported the *cis*-bimetallic complex of dinaphthoporphycene. The interesting part of this complex is that the two palladium metals coordinate to the ligand through the same side. While replacing the acetate with acetylacetonate stabilized an unusual mono-palladium complex of dinaphthoporphycene.<sup>3</sup> Recently, Panda group reported the synthesis of in-core palladium complex using palladium chloride. The crystal structure showed the palladium ion is sitting slightly above the N4 core.<sup>4</sup> Further, their very recent report on the boron complexation of various  $\beta$ -substituted porphycenes, indicated clearly the effect of substituents on the complexation mode in these systems.<sup>5</sup>

In the present study, we wished to replace the  $\beta$ -isopropyl substituents with aryl moieties (endowed with both electron donating and electron withdrawing groups) to explore their effect upon the structure, photophysical and coordination properties.



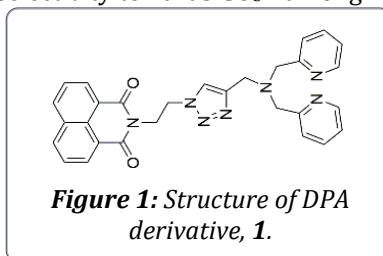
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## PP 20

**Dipicolylamine-Based Fluorescent Probe as a Sensor for Ions and Molecules in Water Milieu**Jinsha K. C.<sup>a</sup>, Ashna Harshad<sup>a</sup>, Roymon Joseph<sup>\*a</sup>*Department of Chemistry, University of Calicut, Thenjipalam, India.**\*roy@uoc.ac.in***Keywords:** Dipicolylamine, Zn<sup>2+</sup> Sensor, Fluorescence *turn-on*, nitroaromatic compounds

Detection of ions and molecules by synthetic receptors is an intriguing area of research owing to the relevance of these species in biology and the environment.<sup>1</sup> Di-(2-picolyl)amine (DPA), is a receptor molecule having many applications in the field of sensing due to the presence of four pyridyl-nitrogen groups that impart chelation towards various metal ions.<sup>2</sup> In the present study, 1,8-naphthalimide has been connected to a DPA molecule through a triazole linker by click reaction to obtain the receptor molecule, **1** (Figure 1). The naphthalimide derivative, **1** shows an excellent selectivity towards Zn<sup>2+</sup> among 11 biologically relevant metal ions as studied by fluorescence spectroscopy in aqueous milieu. The detection of **1** by Zn<sup>2+</sup> has been monitored by a fluorescence *turn-on* mechanism with a fluorescence enhancement fold of ~ 4.5. The selectivity of **1** towards Zn<sup>2+</sup> in the presence of other metal ions was demonstrated by competitive titration wherein Cu<sup>2+</sup> and Ni<sup>2+</sup> only exhibit marginal interferences. Based on the Job's plot analysis, the stoichiometry of the complex formed between the receptor molecule, **1** and Zn<sup>2+</sup> was found to be 1:1. The minimum concentration in which **1** could detect Zn<sup>2+</sup> in a sample by fluorescence spectroscopy was found to be 1.5 × 10<sup>-5</sup> M. The secondary sensing of *in-situ* prepared Zn<sup>2+</sup> complex of **1** (**1.Zn**) towards anions and nitroaromatic compounds has been studied by fluorescence spectroscopy. It has been found that **1.Zn** exhibits selectivity towards CO<sub>3</sub><sup>2-</sup> among 11 anions studied. Further, among 16 nitro compounds, only picric acid and 4-nitroaniline show marginal fluorescence quenching with **1.Zn** indicating the application of **1** in the detection of explosive compounds. The interaction of **1** with Zn<sup>2+</sup> and its secondary sensing applications towards various guest molecules were further supported by UV-visible spectroscopy.

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## An Aggregation Induced Emission Enhancement (AIEE) Fluorescent Probe for the Detection of Copper, derived from 2-Hydroxy-1- Naphthaldehyde and Benzyloxy Benzaldehyde for the Nanoscale Detection of Copper

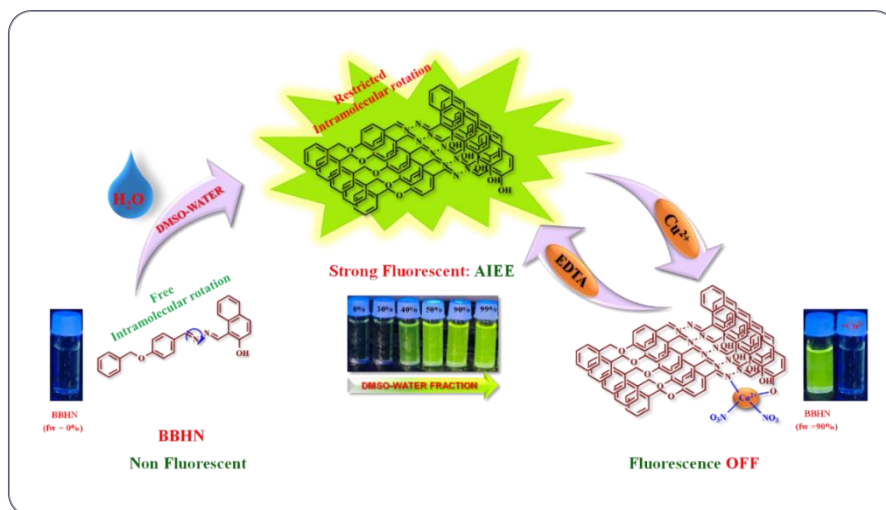
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**Key words:** AIEE, DMSO, dynamic quenching

A novel Schiff base 1-((E)-((E)-(4-(benzyloxy) benzylidene) hydrazono) methyl) naphthalen-2-ol [BBHN] having aggregation induced emission enhancement (AIEE) behaviour in DMSO/Water mixture have been designed, synthesised and characterised using FT-IR, CHNS elemental analysis, HR-MS, <sup>1</sup>H NMR, and <sup>13</sup>C-NMR spectroscopic techniques. The aggregate of BBHN shown relatively high Cu<sup>2+</sup> ion selectivity and sensitivity among various metal ions through fluorescence “turn off” response with very low detection limit of 35.52 nM and a quenching constant value of 2.58×10<sup>8</sup> M<sup>-1</sup>. The results suggested that as synthesised BBHN could effectively function as sensor for the nanomolar detection Cu<sup>2+</sup> ion. Moreover, the fluorescence quenching behaviour of BBHN in presence of Cu<sup>2+</sup> was explained by steady state fluorescence life time measurement study suggests involvement of the dynamic quenching process<sup>1</sup>.



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## PP 22

**Aminoacid Derived Carbon Nanodots for Cold White Led Application**Ritu G.<sup>a</sup>, Renuka N.K.<sup>a\*</sup>*Advanced Material Research Centre, Department of Chemistry, University of Calicut, Malappuram, Kerala, India.**\*renuka@uoc.ac.in***Keywords:** Cold White Led , Self-Quenching Resistance ,CND Powder

Recently, we have seen a substantial rise in research interest in carbon nanodots (CNDs), which are zero-dimensional carbon nanoparticles with size less than 10 nm. Beyond their inherent properties of environmental friendliness, water solubility, electron mobility, and biocompatibility, carbon nanodots (CNDs) are a green nanomaterial with innate luminescence properties, which open up an array of possible applications. Recently these materials have been widely explored for application in light emitting diodes (LEDs)<sup>2,3</sup>. Here we report amino acid derived self-quenching resistant CNDs synthesised via a one pot hydrothermal method, which are suitable for cold white light emitting diode ( cold white LEDs) fabrication. The particles are well characterised using High Resolution Transmission Electronic Microscopy (HR-TEM), X-Ray Diffraction (XRD) analysis, X-ray photoelectron spectroscopy (XPS), Fourier Transform InfraRed Spectroscopy (FTIR), UV-Visible absorbance spectroscopy, and fluorescence spectroscopy. Cold white LED is achieved by simply combining UV LED chips with white light emitting amino acid derived CND powder.

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## From Nanoscale Precision to Macroscopic Impact: Self-Assembled Nanoclusters and Luminescence-Driven Device Fabrication

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**Keywords:** Metal nanoclusters, Self-assembly, Luminescence, Light-emitting diodes, Anticounterfeiting

Atomically precise monolayer thiol-protected noble metal nanoclusters (NCs) emerged as a fascinating area of nanoscience research in the past two decades.<sup>1</sup> NCs are distinct pieces of matter, that possess ultra-small metal cores (< 2 nm), composed of a few to hundreds of atoms protected with a definite number of ligand shells. In the recent past, new and improved protocols were developed to fabricate monodisperse NCs. The molecular composition of monodisperse NCs has been solved by using mass-spectrometry and single-crystal diffraction studies. NCs show size-dependent electronic, optical absorption, photoluminescence, and magnetic properties. NCs have been used as attractive nanoscale building blocks for the fabrication of three-dimensional superstructures via a colloidal self-assembly process. Such self-assembled architectures play an important role in harvesting the enhanced and collective optical properties from the neighbouring NCs. Driving forces such as hydrogen bonding, electrostatic interactions, van der Waals interactions, dipolar interactions, C-H $\cdots$  $\pi$ / $\pi$  $\cdots$  $\pi$  interactions, metal chelation, metal-metal interactions, amphiphilicity, light-triggered dipole-induced interactions, and external templates have been implemented to achieve such assemblies.<sup>2</sup> The organic synthetic toolbox has allowed the rational design of a variety of NCs with specific functional moieties on their surfaces. Particularly, anchoring photoresponsive ligands on the surface of NCs can be utilized as nanoscale building blocks for photoresponsive NC assembly.<sup>3,4</sup> One could foresee that such smart self-assembled superstructures with enhanced photophysical properties are needed to develop future precision devices. The luminescence property of NCs can be efficiently used to probe toxic metal ions/molecules, monitor biological events, production of anticounterfeiting ink,<sup>4</sup> and light-emitting device fabrication.

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## PP 24

Salicylimine-Based Fluorescence Turn-On Sensor for Zn<sup>2+</sup> and Al<sup>3+</sup>

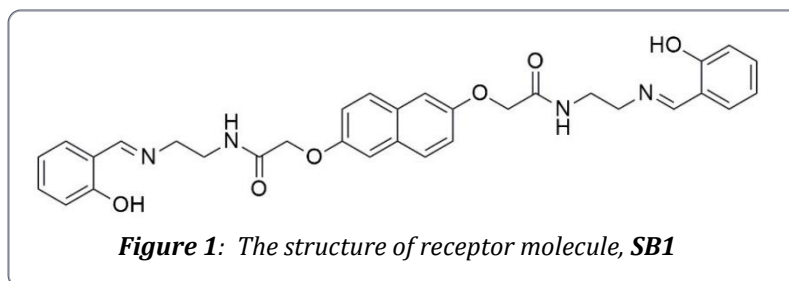
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**Keywords:** Schiff's base, Salicylimine, Fluorescent sensors, Turn-on fluorescence

The detection and quantification of metal ions are paramount owing to their crucial role in various biological processes.<sup>1</sup> For instance, the deficiency and excess of Zn<sup>2+</sup> lead to various diseases such as Alzheimer's, epilepsy, ischemic stroke, infantile diarrhea, etc.<sup>2</sup> Similarly, accumulation of Al<sup>3+</sup> can also result in serious health problems in humans.<sup>3</sup> Hence, it is important to develop sensors for the selective detection of ions having importance in biology. In the present study, a Schiff's base containing salicylimine (**SB1**) has been synthesized and characterized by various spectral techniques such as IR, <sup>1</sup>H, and <sup>13</sup>C NMR spectroscopy (Figure 1). The interaction of **SB1** with 11 biologically relevant metal ions and four toxic metal ions has been studied by UV-visible and fluorescence spectroscopy. The receptor molecule, **SB1**, was found to be selective towards Zn<sup>2+</sup> and Al<sup>3+</sup> among the metal ions, viz.; Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>2+</sup>, Mg<sup>2+</sup>, Mn<sup>2+</sup>, Fe<sup>2+</sup>, Fe<sup>3+</sup>, Co<sup>2+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup>, Cd<sup>2+</sup>, Hg<sup>2+</sup>, and Pb<sup>2+</sup> studied. The Schiff's base **SB1** exhibits turn-on fluorescence with Zn<sup>2+</sup> and Al<sup>3+</sup> with a fluorescence enhancement fold of ~10 and ~20 respectively in methanol. The competitive titration demonstrates the selectivity of **SB1** towards Zn<sup>2+</sup> in the presence of all metal ions except Fe<sup>2+</sup>, Fe<sup>3+</sup>, and Cu<sup>2+</sup>. The interaction of **SB1** with Zn<sup>2+</sup> and Al<sup>3+</sup> has been further supported by UV-visible spectral titrations. The limit of detection of **SB1** was found to be 1.99 x 10<sup>-6</sup> M towards Zn<sup>2+</sup>.

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## Charge Transport Studies of Troger's Base Derivatives in Metal/molecule/Metal Configuration.

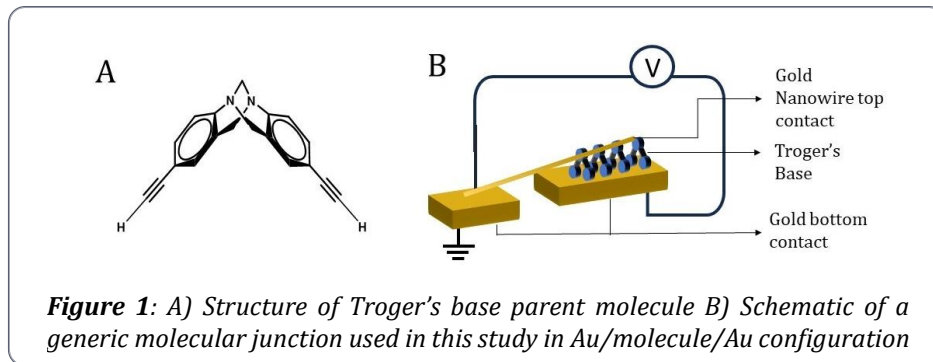
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**Keywords:** Molecular Electronics, Troger's Bases, Charge Transport Properties

The goal of molecular electronics is to use molecules as a functional component element in an integrated circuit.<sup>1,2</sup> The skill of the synthetic chemist in designing molecules with geometric and electronic structures ought to allow the tuning of properties of appropriately designed circuit elements. In this direction we use Troger's bases (Figure 1A) which are V-shaped, chiral, rigid, and C<sub>2</sub>-symmetric molecules,<sup>3</sup> which have been known for long but not been used so far for charge transport measurements. We use a parent Troger's base and its three derivatives for molecular transport measurements in solid state configuration. Here we show a detailed characterization of the self-assembled monolayers of the parent Troger's base and its derivatives on Au surface using techniques such as AFM, XPS, Ellipsometry, Solid-state UV and PMIRRAS. Next, we will measure the current-voltage characteristics of the parent Troger's base and its derivatives in Au/molecule/Au configuration (figure 1B) from 10K to 340K, which will help us to understand the mechanism of charge transport via parent Troger's base and the changes in transport properties with different derivative group.



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## PP 26

**Influence of pH on the Phase Behaviour of Cholesteryl Benzoic Acid at the Interfaces****Veera Manikanta T. N. Moram** <sup>a,b</sup>, P. Viswanath<sup>a\*</sup><sup>a</sup>Centre for Nano and Soft Matter Sciences (CeNS), Shivanapura, Bengaluru, India.<sup>b</sup>Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, India.

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**Keywords:** Langmuir monolayers, phases, pH and textures.

Derivatives of cholesterol and its self-assembly play an essential role<sup>1</sup> in exhibiting liquid crystalline phase, gelators,<sup>1</sup> and also in tear films.<sup>2</sup> It also leads to interesting spatiotemporal behaviour at the air-water (A-W) interface.<sup>3</sup> In this work, we discuss the phase behaviour of the derivative of cholesterol, 4-(6-(cholest-5-ene-3-yloxy)-5-(oxopentyloxy)) benzoic acid (cholesteryl benzoic acid (ChBA)) at the A-W interface<sup>4</sup> and also by adjusting the pH. Surface manometry studies suggest ChBA is highly unstable and tends to collapse early at the A-W interface. For pH (10.5) > pK<sub>a</sub>, ChBA forms a relatively stable film and yields higher collapse pressure. Analysis of the compressional moduli with surface pressure reveals the presence of two phases of different magnitudes (50 mN/m at 20 mN/m and 180 mN/m at 40 mN/m). The textures of the film exhibiting different phases were monitored using a Brewster angle microscope (BAM), which complements surface manometry results. Finding stability of the films, we monitored surface pressure (At, pH-7,10mN/m and pH-11, 10&36mN/m) over time with different pH. We found that at the A-W interface films are unstable when compared to the pH (10.5) > pK<sub>a</sub>.

At the A-W interface, the monolayer of ChBA films was first formed, then it was deposited onto the silicon wafer at a surface pressure of 14 mN/m then we studied using of atomic force microscope (AFM). Topography images show the presence of multi-layers of different thicknesses for ChBA films with a step size of about 2.1 nm. Interestingly, for films deposited at pH > pK<sub>a</sub>, ChBA is primarily seen as a stable uniform monolayer of thickness 3.1 nm. Our study highlights the importance of pH in controlling polar heads' dissociation for obtaining stable ChBA phases at interfaces.

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