

INTERNATIONAL CONFERENCE ON
EMERGING FRONTIERS IN
CHEMICAL SCIENCES
EFCS - 2021

29 – 31 OCTOBER 2021

Inauguration

PROF. N. SATHYAMURTHY

Founder Director, IISER Mohali and Former President, CRSI

Organised by



POSTGRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY

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Preface

The Post Graduate & Research Department of Chemistry, Farook College (Autonomous) is very pleased to release the Book of Abstract of the International Conference on “ Emerging Frontiers in Chemical Sciences, EFCS-2021” conducted during October 29-31, 2021. This volume is an account of most of the contributions presented at the conference.

EFCS-2021 is the third international event in the EFCS conference series hosted by Farook College with a view to provide a platform for young researchers and science aspirants to communicate with international and national experts. This event is very rich with the participation of eminent scientists of international and national reputation. The most respected Prof. N. Sathyamurthy, Indian Institute of Science Education and Research Mohali, is the inaugural speaker of EFCS 2021. Another attraction of the conference is the honouring ceremony of Prof. K. K. Unnikrishnan, Retired Professor, Farook College by EFCS Life Time Achievement Award for his outstanding service to academics and society. The EFCS committee also recognise the efforts of young researchers by honouring with EFCS Young Scientist Award and Dr. Tania Francis, Assistant Professor, St. Joseph College, Devagiri is selected for this recognition.

We would like to thank all the academicians, delegates and participants for their contributions to the Conference. We are much grateful to the sponsors of the programme including RUSA, University Grants Commission, M/s Ambernath Organics Pvt Ltd., Mumbai and the College Managing Committee.

In this volume, abstracts of invited lectures are given at the beginning, followed by abstracts of papers presented at the conference. The editorial board has tried its level best to make this collection a comprehensive one. This book of abstracts presents a snapshot of the state of development other subject at the time and would be invaluable for that reason.

We thank all those who have contributed to the successful organisation of the conference.

October 29-31, 2021

Organising Committee
EFCS 2021

EFCS 2021

29-31 October 2021

Day 1 - 29th October 2021, Friday

Inaugural Session

9.00 AM: : **Chief Guest: Prof. N. Sathyamurthy**
Honorary Professor and Former Director, Indian Institute of Science Education and Research Mohali, Former President, Chemical Research Society of India.

Honouring: Prof. K. K. Unnikrishnan
(Life time achievement award)

Dr. Tania Francis
(Young Scientist Award)

Technical Session 1

10.10 AM **The Beginning of Chemistry**

Prof. N. Sathyamurthy
Honorary Professor and Former Director, Indian Institute of Science Education and Research Mohali, Former President, Chemical Research Society of India.

10.50 AM : **Droplet Synthesis**

Prof. T. Pradeep
Indian Institute of Technology Madras

11.30 AM – 11.40 AM : **Break**

Technical Session 2

11.40 AM : **What is so interesting about $MA_{1-y}FA_yPbX_3$**

Prof. D. D. Sarma
Indian Institute of Science Bangalore

12.20 PM **Chemically Modified Gold Superatoms**

Prof. Tatsuya Tsukuda
University of Tokyo, Japan

1.00 PM – 2.00 PM **Break**

2.00 PM – 3. 15 PM **Paper presentations**

3.30 PM	Technical Session 3 Hard-Soft Gate Control to Tune Dynamicity of a Family of MOFs Prof. R. Vaidhyanathan <i>Indian Institute of Science Education and Research Pune</i>
4.10 PM	Responsive DNA Nanostructures for Cancer Therapy Prof. Reji Varghese <i>Indian Institute of Science Education and Research Thiruvananthapuram</i>
5.00 PM – 5.10 PM	Break
5.10 PM – 6.40 PM	Technical Session 4 Paper Presentations
	Day 2 - 30th October 2021, Saturday
9.00 AM	Technical Session 5 Electrospray Gold Standards -Viruslike Clusters I-197Au144-5 Prof. Robert Lloyd Whetten <i>Northern Arizona University, USA</i>
9.40 AM	Interfacial Electrochemical Studies Using Layered Chalcogenides, Transition Metal Nitrides and Carbides Prof. S. Sampath <i>Indian Institute of Science Bangalore</i>
10.20 AM	Pb-Free Metal Halide Perovskites Prof. Angshuman Nag <i>Indian Institute of Science Education and Research Pune</i>
11.00 AM - 11.10 AM	Break
11.10 AM	Technical Session 6 The Quest for Robust Superhydrophobic Surfaces Prof. Robin Ras <i>Aalto University, Finland</i>
11.50 AM	Cavity Catalysis: A New Route to Control

	Chemical Reactions Dr. Jino George <i>Indian Institute of Science Education and Research Mohali</i>
12.30 PM - 1.30 PM	Break
1.30 PM – 2. 45 PM	Paper presentations Technical Session 7
3.00 PM	Role of the African Academy of Sciences in Promoting Research Partnerships between Global South & North Prof. Jane Catherine Ngila <i>The African Academy of Sciences, Kenya</i>
3.40 PM	π-Conjugated Polymers in Energy Applications Prof. Asha S. K <i>CSIR - National Chemical Laboratory, Pune</i>
4.20 PM	Computational Modelling of Atomic Clusters Prof. Anoop Ayyappan <i>Indian Institute of Technology Kharagpur</i>
5.00 PM – 5.10 PM	Break
5.10 PM	Technical Session 8 Precisely Engineered Peptide-Derived Transmembrane Ion Transporters for Enhanced Ion Selectivity Prof. Nandita Madhavan <i>Indian Institute of Technology Bombay</i>
5.50 PM	Organocatalysis Using N-Heterocyclic Carbenes (NHCs) Prof. Akkattu T Biju <i>Indian Institute of Science Bangalore</i>
6.30 PM	Process Research and Process Development in Agro Chemical Active Ingredient (AI) Development Dr. Bhanu Manjunath <i>Director Research and Technology Centre, Syngenta Biosciences Pvt Ltd, Goa</i>

Day 3 - 31st October 2021, Sunday

- 9.00 AM** **Technical Session 9**
Topic - Total Synthesis of Metallic Molecules
Prof. Jianping Xie
National University of Singapore, Singapore
- 9.40 AM** **Topic - Bismuth Halide Perovskites: Organic**
Spacer Cations Induced Modulation of
Optoelectronic Properties
Dr. Vijayakumar C. Nair
CSIR-National Institute for Interdisciplinary
Science and Technology, Thiruvananthapuram
- 10.20 AM – 10.30 AM** **Break**
- 10.30 AM** **Technical Session 6**
Topic - Gas Separation Performance of Mixed
Matrix Membranes Based on Poly Vinyl
Alcohol and Polyhedral
Oligomeric Silsesquioxane
Dr. Ranimol Stephen
St. Joseph College Devagiri, Calicut
- 11.10 AM:**
Topic - Computational Insights on the
Unprecedented Catalytic Reactions
Dr. Rositha Kuniyil
Indian Institute of Technology Palakkad
- 11.50 AM -12.30 PM** **Valedictory Session**
- 12.30 PM - 1.30 PM** **Alumni Meet**

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The Beginning of Chemistry

N. Sathyamurthy

Honorary Professor, IISER Mohali

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Abstract: From what we understand from the astrophysicists and the Big Bang theory of the beginning of the universe, the first element to be formed in the universe was helium, followed by hydrogen and lithium in the ratio 0.1, 1 and 10^{-10} , respectively. It appears that the first chemical bond to be formed was between He and H^+ by radiative association. This was followed by the formation of H_2^+ and H_2 through processes such as $HeH^+ + H \rightarrow He + H_2^+$; $H_2^+ + H \rightarrow H_2 + H^+$. Triatomic species like H_3^+ were formed too: $HeH^+ + H_2 \rightarrow He + H_3^+$. After a brief introduction to some of the events that took place in the early universe, the dynamics of $He + H_2^+ \rightarrow HeH^+ + H$; $He + H + H^+$ reactions would be presented from classical and quantum mechanical points of view. The system is rich in conical intersections. The possibility of HeH_2^+ formation due to the nonadiabatic coupling acting as frictional force will also be discussed.

Droplet Synthesis

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Abstract: Micrometer size droplets formed in electrospray can be used for chemical synthesis.^{1,2} In this lecture, I will present new possibilities in the synthesis of molecules,³ nanoparticles^{4,5,6} and assemblies of nanostructures^{7,8}. These methods will be explored further to understand the chemistry of nanoparticles in droplets. In very recent experiments, our group has explored diverse tools of imaging to understand the anisotropic distributions of molecules and nanoparticles in such droplets. I will conclude the lecture with examples of very recent research in which we explored the chemistry at the surface of droplets as they move through a medium.

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What is so interesting about $\text{MA}_{1-y}\text{FA}_y\text{PbX}_3$

D. D. Sarma

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Abstract: The last decade has seen the most spectacular rise of the halide perovskites with the general formula of ABX_3 , where most commonly $A = (\text{CH}_3\text{NH}_3)^+$ (MA), $(\text{CH}(\text{NH}_2)_2)^+$ (FA) or Cs^+ , $B = \text{Pb}^{2+}$ or Sn^{2+} , and $X = \text{I}$, Br or Cl for their superlative photovoltaic and light emissive properties. MAPbI_3 is the most investigated among the pure systems. However, a rapid degradation of its performance has been a vexing issue, ameliorated by A -site cationic substitutions, such as in $\text{MA}_{1-y}\text{FA}_y\text{PbX}_3$. However, the microscopic changes brought about by such substitutions are not well understood at present. We address these issues by first making a comparative study of the pure end-members, MAPbX_3 and FAPbX_3 to understand their distinctive features at some fundamental levels, such as the dielectric properties¹ and the rotational dynamics² of these two organic moieties from quasi-elastic neutron scattering experiments. We then investigated³ the substitutional series, $\text{MA}_{1-y}\text{FA}_y\text{PbI}_3$, for a range of compositions (y) and over a wide temperature range to map out the structural phase diagram in the temperature–composition phase space, identifying four crystallographic phases. Temperature and frequency dependent dielectric measurements show remarkable dependency of dielectric properties on the specific crystal structures; significantly, it is seen that the presence of FA ions hinder the nearly-free rotations of the MA units, giving rise to a glassy dipolar state. We also find evidence of a systematically enhanced stability on doping of FA from our analysis of the temperature dependent photoluminescence from this solid solution with different composition, y .⁴

This work is a result of several collaborations with C De, J. P. Embs, TN Guru Row, A Hossain, BP Kore, A Mohanty, R. Mukhopadhyay, Sharada G, V. K. Sharma, D Swain, and M. Tyagi.

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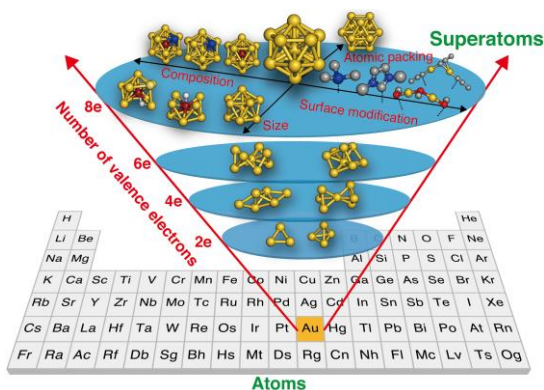
Chemically Modified Gold Superatoms

Tatsuya Tsukuda

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Abstract: Gold clusters, consisting of a few to a hundred gold atoms, have attracted growing attention as building units of novel functional materials because they exhibit unique physicochemical properties due to their discrete electronic structures and non-FCC atomic packing structures. Recent progress in atomically precise synthesis, X-ray crystallography and theoretical calculations¹ has revealed that the ligand-protected Au clusters can be viewed as “chemically modified Au superatoms” owing to the atom-like electronic shell structures. For example, the magic stability of the icosahedral M@Au₁₂ core is associated with a closed electron configuration (1S)²(1P)⁶, similarly to that of noble gases. A unique feature of the superatoms compared to the conventional atoms is that their properties can be controlled by a variety of factors such as the number



of constituent atoms, composition, shape, and surface modification.^{2,3} We are trying to systematize superatoms as artificial elements at the nanoscale in the form of a periodic table (Fig. 1). In this talk, I will discuss the correlation between the structures and properties of these superatoms^{4,5} and introduce chemical transformations for the synthesis of higher-order structures such as pseudo-molecules of superatoms (superatom molecules).^{6,7}

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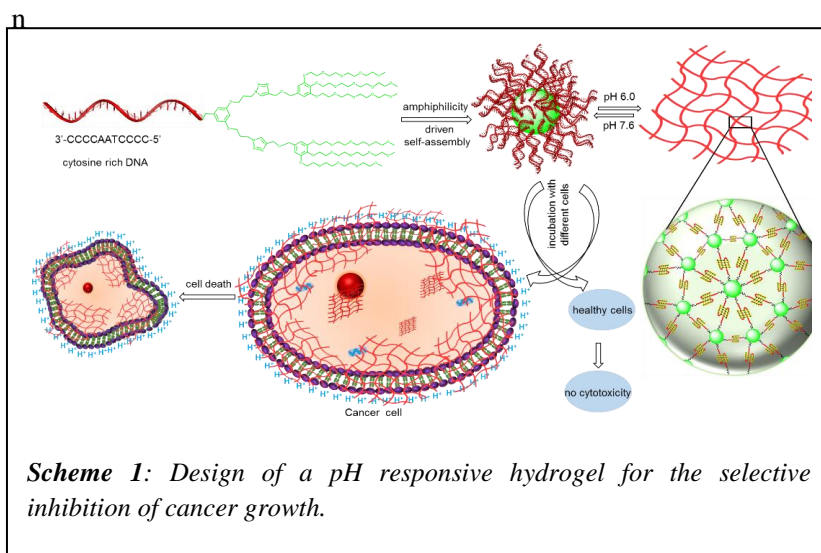
Responsive DNA Nanostructures for Cancer Therapy

Reji Varghese

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Abstract: Improving the effectiveness of the anticancer drugs while minimizing their side effects is a great challenge in cancer research. Recent research efforts in this direction have shown that encapsulating the cell in a gel network can lead to the cell death. Considering the high proton gradient along the cancer cells membrane, we have designed a pH responsive DNA based smart material which contains C-rich DNA as hydrophilic domain and glycol dendron as a hydrophobic domain, which will self-assemble into micellar nanostructure in basic environment, on acidification cytosine gets protonated and forms inter molecular i-motif, which brings them together and leads to the formation of entangled



networks could entrap water molecule which leads to the formation hydrogel. The pH triggered i-motif formation and the fusion of the micelles have been characterized using different spectroscopic and microscopic analysis. The hypothesis was examined using three different cell lines, HeLa, A549 and HEK, where HeLa and A549

cell lines are cancer cell line and HEK is healthy cell line. MTT assay analysis reveals that pH responsive hydrogel is highly cytotoxic for the cancer cell lines and biocompatible for the healthy cell lines. Moreover, CLSM analysis on HeLa cell line showed an extra cellular gelation. Our results suggested that pH responsive hydrogel is a good candidate for the selective inhibition of cancer growth (Scheme 1). Details of these results will be presented.

Electrospray Gold Standards of Molecular Mass 32- to 52-kDa: Charging Patterns of the Ubiquitous Viruslike Clusters, $I - {}^{197}\text{Au}_{144.5}(\text{SR})_{60}$, $R = 9$ Variants, in Native [HPLC]-ESI-MS Short title: Electrospray Gold Standards -Viruslike Clusters $I - {}^{197}\text{Au}_{144.5}$

Robert L Whetten

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Abstract: Faraday's legendary 'Molecules of Gold' have stimulated intense interest (over 165 years) but have only recently begun to yield their secrets to modern methods of chemical analysis. Here(in), we demonstrate how striking charging patterns emerge directly from native electrospray of large, gold-rich molecules that were generated by reduction of various (9) small gold(I)thiolate complexes [-RS-Au(I)-SR-], followed by extensive thermochemical processing to enrich the most robust forms. In each case (R), electrospray ionization of a picomolar solution yields a characteristic series of intense, highly resolved peaks at related (m/z)-ratios, that can be used to deduce charges $\{z e^+\}$ and hence a distinct molecular mass, $\{M_R\}$. A plot of $\{M_R\}$ versus thiolate-mass $\{mR\}$ yields a straight line with slope 60.0 (the ligand count) and an intercept of 28,364-Da, the mass of 144 Au-atoms. i.e. an unique molecular composition $\{{}^{197}\text{Au}_{144}(\text{SR})_{60}\}$. This formula agrees with the unique chiral - icosahedral structure -mode, $c@12@42@60@(30,60)$, the $\text{Pd}_{145}(\text{CO})_{60}$ -structure, that features a massively-compact globular Au_{114} -core ($\sim 1.6\text{-nm}$) and an intrinsically chiral (I) outer shell ($\sim 2.0\text{-nm}$) with 60- fold site equivalence, denoted by Martin *et al.* as 'viruslike' on the basis of its resemblance of icosahedral-virus capsids. The charging patterns are interpreted within this model as characteristic of the R -group class. The mass-fraction of the isotopically-pure ${}^{197}\text{Au}_{144}$ ranges from a high 88.6% ($R = \text{C}_2\text{H}_5$) down to $\sim 60\%$ (PEGylated and quaternized R groups). The remarkable set of features discussed herein suggests that these ubiquitous, robust, viruslike molecules-of-gold may serve an important function as widely available high-performance standards for high-resolution metrology, which goal stipulates specific benchmarks for further development and extensions.

Interfacial Electrochemical Studies Using Layered Chalcogenides, Transition Metal Nitrides and Carbides

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Electrochemical interfacial studies have gained enormous attention in the recent past especially due to interest in energy conversion and storage. This calls for efficient catalysts for various redox reactions involving small molecules. Our group has been working on various materials in this direction. The present lecture will describe some of our efforts based on two-dimensional layered materials, transition metal nitrides and carbides. They are interesting systems for electrocatalysis, energy storage and solid-state devices due to their favourable physicochemical properties that can be attained by varying the composition and thickness. Small molecules including hydrogen, oxygen, methanol are ones of interest at present. Using the fundamental knowledge, it is possible to further delve into applications based on energy storage, such as batteries, capacitors and fuel cells. The present lecture will discuss results from our group in the above mentioned areas.

Pb-Free Metal Halide Perovskites

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Abstract: Lead (Pb) halide based perovskites show outstanding optoelectronic properties. But Pb-toxicity remains an issue for their widespread application. For example, Pb content in electronic products is restricted to 0.1 wt% by the European Union guidelines. Therefore, search for Pb-free metal halide perovskites is natural. The fundamental question is how to identify alternative metal halides that could replicate optoelectronic properties of the Pb-halide perovskites.^{1,2} I will address this question in the first part of my talk. Unfortunately, till date, Pb-free perovskites could not compete with optoelectronic properties Pb-halide perovskites. Why so? This question will also be discussed in my talk. Finally, in the last 2-3 years, we changed the goal post of our research. Instead of attempting to replicate the optoelectronic properties of Pb-halide perovskites, we started to explore newer directions. For example, we dope lanthanides like Yb and Er in Cs₂AgInCl₆ double perovskites to develop short-wave-infrared (SWIR) light emitting materials.³ Furthermore, doping and/or codoping ions like Bi³⁺ and Sb³⁺ (that has two electrons in the outermost s-orbital) tailor both optical excitation and emission in the UV-visible region.^{4,5} In the last part of my talk, I will discuss about such exploration.

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The Quest for Robust Superhydrophobic Surfaces

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Abstract: Nature offers various examples of extreme water-repellency, such as the leaves of Lotus plant and wings of cicada. The water repellency allows plants for efficient photosynthesis even in dusty environments, and allows large-wing insects to fly even in humid conditions. Likewise, our technological society could benefit from surfaces that stay clean and dry in challenging conditions. For example, solar cells on roof tops lose efficiency when they are covered with sand and dust. The extreme water-repellency, also called superhydrophobicity, is attributed to the combination of micro/nanoscale topography and hydrophobic surface chemistry that allows trapping of a thin air film between the water and the solid substrate. The air film effectively shields the water from the solid by reducing the contact area, leading to very high contact angle and very low adhesion and friction. The required topography, however, also makes these surfaces very fragile.

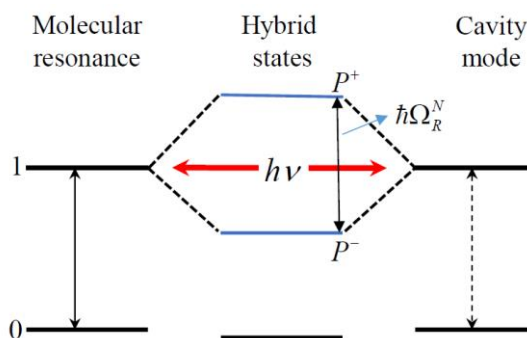
Here I will present the progress made during previous decade, including different strategies for enhancing the mechanical durability. Recently, in collaboration with the group of Xu Deng, we developed an extremely durable superhydrophobic surface, by making use of a microstructured armor that protects the otherwise fragile nanostructures. I will present the concept, and steps that we are taking towards commercialization.

Cavity Catalysis: A New Route to Control Chemical Reactions

Jino George

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Abstract: Vibrational strong coupling (VSC) is an unconventional technique to control chemical reactions very precisely by targeting a vibrational state.¹ VSC generate hybrid states by coupling a vibrational state to an infrared cavity mode (**Scheme 1**). This process reshuffles the energy of the reacting species. We catalyzed a simple ester hydrolysis process by VSC of C=O band of the ester in a flow cell Fabry-Perot cavity. Thermodynamic studies suggest that the enthalpy and entropy of activation are modified under VSC conditions. In another attempt, large biomolecules such as alpha-chymotrypsin



Scheme 1: Light-matter strong coupling of a molecular state and a cavity mode.

is coupled to the vacuum field via VSC of water.² In this case, we improved the enzyme catalysis process and found that cavity coupling can bring a competitive enhancement in the reaction. The two important features of cavity catalysis are high sensitivity with cavity tuning and increase in the reaction rate with increasing coupling strength. A series of experiments conducted in different derivatives of an ester suggests the breaking of the linear free-energy relationship.³ Our recent findings are in agreement with the non-linear behavior observed spectroscopically.⁴ Cavity catalysis is purely an unconventional way of controlling chemical reactions that will have direct application in chemistry.

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Role of the African Academy of Sciences in Promoting Research Partnerships between Global South & North

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Abstract: The African Academy of Sciences (AAS) is a non-aligned, non-political, not-for-profit pan African organisation whose vision is to see transformed lives on the African continent through science. AAS has tripartite mandate namely, recognising excellence through the highly prestigious fellowship and award schemes, providing advisory and think tank functions for shaping the Africa's Continental Science, Technology and Innovation (STI) strategies and policies and implementing key STI programmes addressing Africa's developmental challenges. AAS has five strategic focus areas: Environment and climate change, health and wellbeing, natural sciences, policy and governance, and social sciences and humanities. The slightly more than 500 AAS Fellows, who are elected based on their publication record, innovation, leadership roles and contribution to policy, provide the strategic leadership to shape continental programmes, engage with governments to enable wise investment on the continent, serving as reviewers for grant applications and mentor early career scientists. The AAS also awards the Obasanjo Prize every two years to an outstanding scientist who contributes to the development of the continent.

The AAS Activities and Networks both with Global South and North are achieved through these platforms; (i) Funding and Agenda Setting through Alliance for Accelerating Excellence in Science in Africa, which is a business wing of the Academy aimed at funding research projects; (ii) Publishing Platforms (AAS Open)- AAS Open Research is an innovative open access platform to enable the African Academy of Sciences' funded and affiliated researchers to publish immediately, without barriers and with the benefit of

transparent peer review process; (iii) Good Financial Grant Practice in partnership with Global Grant Community (GGC) with a mission to allow financial management using the disruptive power of technology to digitize, standardize and de-risk the due diligence process for both funders and grant receivers; (iv) Coalition for Africa Research and Innovation as a sustainability platform set up partnership with regional and global partners; (v) Africa's Scientific Priorities programme that engages Africa's science leaders and political stakeholders to identify top scientific priorities, to offer the highest return on investment for Africa's sustainable development, through top ten scientific priorities for Africa; (vi) Evidence Leaders in Africa aimed at expanding leadership to use evidence based science research and innovation for policy formulation and implementation by African governments for the good of communities.

Computational Modelling of Atomic Clusters

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Abstract: Atomic cluster is an ensemble of bound atoms or molecules, intermediate in size between a simple molecule and a nanoparticle up to a few nanometers in diameter. The most exciting feature of atomic clusters is that their properties evolve as a function of size from single atom to the bulk. Determining the geometries of atomic clusters is crucial for understanding this phenomenon. Computational modelling can help us to identify several possible geometries including the most stable one - the global minima. Global optimization techniques are used for exploring the complex potential energy surface of atomic clusters. The methods commonly used in predicting the geometries, examples of such systems, and their properties will be discussed.

Precisely Engineered Peptide-Derived Transmembrane Ion Transporters for Enhanced Ion Selectivity

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Abstract: Transmembrane ion-transport mediated by carriers and channels is crucial for the smooth functioning of living organisms. Synthetic transporters that mimic transmembrane ion transport are potential drugs for diseases related to ion-channel dysfunction. Molecules that mimic the gating behavior of ion channels can also be exploited to develop molecular switches and sensors. Peptides with their rich functional group diversity and biocompatibility are attractive scaffolds for the aforementioned applications. We have developed a tool kit for selective transmembrane transport using a readily accessible universal peptide scaffold and suitable “selectivity inducers”. We have also designed macrocyclic scaffolds that can potentially be used for regulated ion-transport. The talk will summarize our efforts towards engineering ion-selective and regulated transmembrane transport.

Organocatalysis Using N-Heterocyclic Carbenes (NHCs)

A. T. Biju

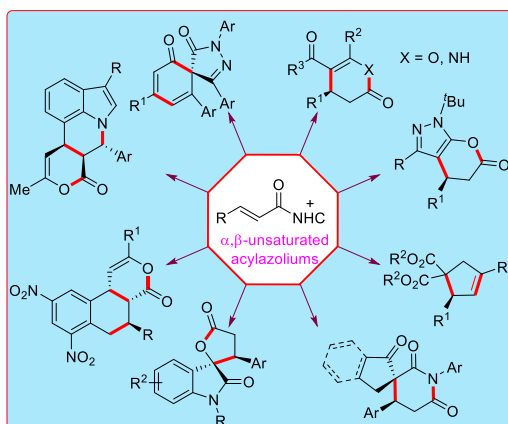
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Catalysis is a fundamentally sustainable process, which can be used to produce a wide range of chemicals and their intermediates. Among the various catalytic methods, N-heterocyclic carbene (NHC)-catalyzed umpolung of aldehydes is widely used for the unconventional access to target molecules.^[1] Moreover, NHC-

catalysis is known for umpolung of Michael acceptors, but imine umpolung was unknown in this realm of catalysis. In this context, we have demonstrated, for the first time, the NHC-catalyzed umpolung of imines for the synthesis of 2,3-disubstituted indoles, functionalized



quinolines and dihydroquinoxalines.^[2] In addition, NHC-catalysis is widely used for the generation of α,β -unsaturated acylazoliums followed by their interception with various nucleophiles, the formal [3+3] annulation reactions. In this area, recently we have reported the enantioselective NHC-catalyzed annulation reactions for the synthesis of dihydropyranones, dihydropyridinones, cyclopentenes, pyrazoles, spirocyclohexadienones, tricyclic \square -lactones, tetracyclic indoles etc., where NHC-bound α,β -unsaturated acylazoliums are the key intermediates.^[3] Very recently, we employed the umpolung of aldehydes for the synthesis of axially chiral C-N bond-containing molecules.^[4] The details of these works will be presented.

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Process Research and Process Development in Agro Chemical Active Ingredient (AI) Development

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Abstract: Agrochemicals are small molecules which need to be manufactured in large quantities (5000 to 50,000 tons/year) to cater to the demands of the global market. Chemistries for synthesis of these molecules need to be very robust, safe, and sustainable. The way process research and development teams enable companies to develop unique routes and technology to ensure the compounds are manufactured in the a right manner will be highlighted

Total Synthesis of Metallic Molecules

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Abstract: Total synthesis, where desired organic- and/or bio-molecules can be produced from simple precursors at atomic precision and with known step-by-step reactions, has prompted centuries-lasting bloom of organic chemistry since its conceptualization in 1828 (Wöhler synthesis of urea). Such expressive science is also highly desirable in nanoscience, since it represents a decisive step towards atom-by-atom customization of nanomaterials for basic and applied research. Although total synthesis chemistry is less established in nanoscience, recent years have witnessed seminal advances and increasing research efforts devoted into this field. In this talk, I will discuss our recent work on introducing and developing total synthesis routes and mechanisms for atomically precise metal nanoclusters. Due to their molecular like formula and properties (e.g., HOMO-LUMO transition, strong luminescence and stereochemical activity), atomically precise metal NCs could be regarded as “metallic molecules”, holding potential applications in various practical sectors such as biomedicine, energy, catalysis and many others. More importantly, the molecular-like properties of metal nanoclusters are sensitively dictated by their size and composition, suggesting total synthesis of them as an indispensable basis for reliably realizing their practical applications.

Bismuth Halide Perovskites: Organic Spacer Cations Induced Modulation of Optoelectronic Properties

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Abstract: Lead halide perovskites attract significant research interest due to their potential for high-efficiency and cost-effective optoelectronic devices. The unique photonic and electronic properties of these materials brought them to the forefront of materials science research. However, the high toxicity and poor stability of lead-based perovskites are the major hurdles for their commercialization. These issues triggered a considerable effort for the development of stable and environment-friendly lead-free perovskites. In this context, bismuth halide perovskites (BHPs) were found to be ideal rivals for lead-based materials owing to their excellent chemical stability, less toxicity, and structural versatility. Understanding the crystal structure and optoelectronic properties of BHPs is crucial for designing them for specific, tailor-made, functional devices. We have used a comprehensive experimental and theoretical investigation to probe the optical and electronic properties of BHPs. Our findings on the structure-optoelectronic property correlations provide a guideline to the rational selection of organic spacer cations in designing BHPs featuring low exciton binding energy, narrow optical band gap, enhanced visible light absorption, and high photoconductivity. One of our key observations is that by increasing the electron affinity of the organic spacer ligands, photoconductivity and visible light absorption of BHPs could be significantly enhanced. Details of our findings will be presented.

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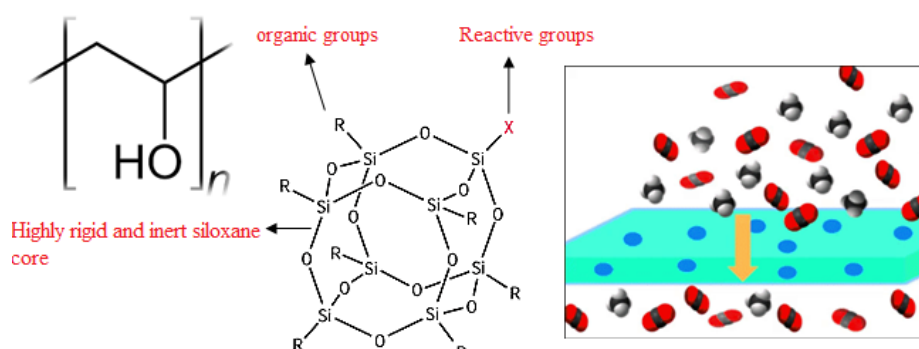
Gas Separation Performance of Mixed Matrix Membranes Based on Poly Vinyl Alcohol and Polyhedral Oligomeric Silsesquioxane

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Abstract: Membrane separation technology is a low cost and energy efficient method for separation of gases, vapours, liquid mixtures and azeotropic mixtures. The main challenge in membrane separation technology is to overcome the trade-off effect between permeability and selectivity. In order to tackle this problem, one promising strategy is the introduction of fillers to get mixed matrix membranes (MMMs). MMMs can be developed using conventional fillers, nano fillers, metal organic frameworks(MOFs) and covalent organic frameworks (COFs). It is difficult to prepare defect free MOFs membranes and hence MMMs find application in separation process. Major challenge in the fabrication of polymer/MOF membrane is in the interfacial interaction between the organic polymer phase and the MOF phase. When compared to MOFs, COFs shows less selectivity owing to its larger pores and the lack of metal sites in the framework. However, COFs



shows higher selectivities than zeolites and activated carbon. Gas separation is important in chemical industries for product isolation, recovery of reactants and in pollution control. The first large industrial scale application of gas membrane was launched by the company Permea for hydrogen separation

from purge gas streams of ammonia plants. The presentation is on the applications of polymer membranes and MMMs in the separation of gases followed by the findings obtained for poly(vinyl alcohol)/ polyhedral oligomeric silsesquioxane (POSS) MMMs. Polyhedral oligomeric silsesquioxane (POSS) is an inorganic- organic hybrid nanomaterial, used to improve the properties of polymeric systems. The inorganic component is a rigid siloxane core and can be decorated with various organic functional groups to enhance the compatibility with polymers.

Computational Insights on the Unprecedented Catalytic Reactions

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Abstract: With the emergence of new synthetic strategies in catalysis comes the need for mechanistic studies, which can help rationalize the outcomes and thus enable improvement in future reaction scheme design.¹ To this end, the computation of transition state models using Density Functional Theory (DFT) is an established method of choice for the mechanistic elucidation of a wide array of regio- and stereoselective reactions.² These approaches recently allowed for the evaluation of significantly larger chemical space in transition metal catalysis that would represent a major synthetic challenge for novel catalyst design.³

This talk will outline the detailed mechanistic understanding of various unprecedented reactions.⁴ To this end, I will present the strategies I have applied during the past few years for the elucidation of mechanisms of the C–H arylation and decarboxylation reactions. The detailed chemical insights in the presentation will unravel the identification of photocatalytically active species, the importance of additives, and factors controlling the origin of selectivity by employing DFT and TD-DFT methods. Furthermore, how these obtained insights and methods can be proposed to apply in the future for refining the transition state models for the dispersion enabled catalyst design and the directed evolution employed artificial metalloenzyme design will be discussed. The key focus of the presentation is the efficient use of the synergy between the theory and experiment to overcome the current inherent challenges for novel catalytic design.

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PRESENTATIONS

Expanding Purview of 3D-printing Technology towards Multidimensional Applications

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Abstract: 3D-printing or additive manufacturing (AM) is an evolving field of technology, known for its rapid, scalable and advanced manufacturing technique for electrode fabrication.¹ The technology has now started to find multiple applications in several domains within a short period of time, owing to its print-on-demand facility that can print any prototype. The printed electrodes are suitably treated and used for targeted applications. The metal plating of 3D-printed carbon electrodes (3D-CE) using copper and nickel is one such approach towards electrochemical sensing of carbohydrates sugars.² In another work, these electrode surfaces were modified for electrocatalytic reactions, such as hydrogen evolution reactions, via dip coating technique. The activated electrode surfaces were ideally dip coated using 2D materials such as, transition metal dichalcogenides (TMDs), and MXenes. This showed the possibilities to design substrates that are simple, and cost effective over other complex conventional techniques.³ 3D-printing of 2D materials such as MXenes are also gaining significant attention. Also, 3D-printing proved to be highly advantageous during the breakdown of the ongoing COVID-19 pandemic, especially for mitigating the shortage of protective equipment in the health sector.⁴ In short, we conclude that 3D-printing is a highly promising technology with significant scope in the future, to fulfil the needs of day-to-day life.

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Formation of Ultrathin Nanosheets via DNA Assisted Assembly of Amphiphilic Fullerene Derivative

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Abstract: DNA, a versatile template for the organization of functional moieties, draw great attention in the fields of biomedicine,³nanoelectronics⁴ etc. due to its unique structure and sequence programmability.^{1,2}Non-covalent interactions such as electrostatic interaction with the phosphate backbone, major or minor groove binding and intercalation within the nucleobases majorly contribute to the assembly of functional entities within the DNA architecture. But the precise organization of small molecules often require covalent modification of DNA and demand more sophisticated methods and expertise. Herein, we have achieved DNA assisted, long range, ordered assembly of fullerenes leading to micrometer sized ultrathin nanosheets through a facile non-covalent approach using a cationic fullerene amphiphile (**FPy**) and various DNA structures. Longer duplex DNAs such as linear λ -DNA and circular pBR322 plasmid DNA readily condense in presence of **FPy** to form nanosheet structures with sub-micrometer lateral dimensions. On the other hand, short single strand and double strand DNAs form extended nanosheets with significantly higher crystallinity. DNA condensation and subsequent self-assembly were probed using UV-visible absorption spectroscopy, while morphological changes upon DNA/**FPy** assembly were studied through AFM and TEM techniques. The presented strategy is useful for applications such as gene delivery and for constructing DNA based nanostructures. Details of synthesis of fullerene derivatives, photophysical and morphological characterization of the self-assembled nanostructures and structure-property relationships will be discussed during this presentation.

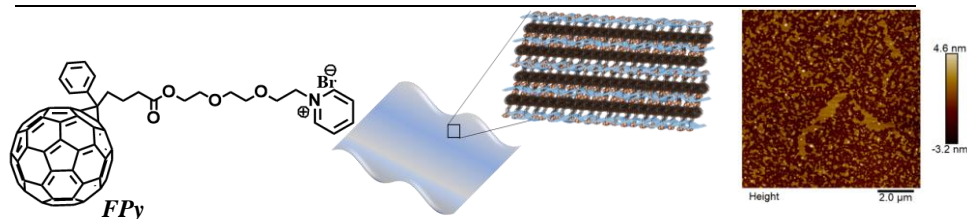


Figure 1. Schematic representation and AFM image of **FPy**/DNA assembly

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Controlled Synthesis of Hematite Nanostructures & Its Composites for Photocatalytic, Photocurrent and Battery Material Applications

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Abstract: We report the template assisted synthesis of controlled self-assembly nanostructures such as nanorods (1D), hexagonal platelets (2D), and spheres (3D). 0D particles were synthesized adopting auto-combustion method using kalonji seeds as a green fuel for the first time. Effect of precipitating reagent, capping agent, residence time in the autoclave on phase and particle size while synthesizing nanostructures were thoroughly studied. Composites of Hematite-Hausmanite, Hematite – Cuprous Oxide were obtained through hydrothermal synthesis. The synthesized metal oxide nanostructures and the composites were characterized for phase purity and crystallographic properties using X-Ray powder diffraction. Profile matching and Rietveld refinement was performed using Full PROF software to know the quantitative phase analysis and atomic positions. Pair Distribution Function analysis (PDF) was performed to understand the vacancy ordering of the material due to the reduction in particle size. The bandgap of the synthesized materials was evaluated through DRS. Morphological studies were performed using SEM. Systematic photocatalytic degradation using the metal oxides and composites as catalysts were demonstrated using low power visible light in a customized catalytic reactor. 90% degradation of Rhodamine B was recorded under a 50W visible lamp. ITO glass substrate was adopted to test the photocurrent properties. Electrochemical performance of 0D and 3D are compared through charge-discharge cycles. 0D nanoparticles showed better photocatalytic activity owing to the high surface area, while 3D nanospheres showed better battery performance.

Light-Emitting Atomically Precise Nanocluster-Based Flexible QR Codes for Anticounterfeiting

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Abstract: Counterfeiting of any official documents, especially currency, passport, stamp, and so forth, is a global concern that affects the security and revenue of a country. Although many of these are protected with anticounterfeiting techniques, the estimated global economic loss due to duplication has been increased significantly and reached up to multibillion USD per annum. Despite tremendous progress in the field of fluorescence-based anticounterfeiting, the advanced anticounterfeiting techniques are still posing challenges all over the world due to their cost and reliability. Recently, light-emitting atomically precise nanoclusters have emerged as attractive building blocks because of their well-defined structure, function, and stable photoluminescence.¹⁻⁵

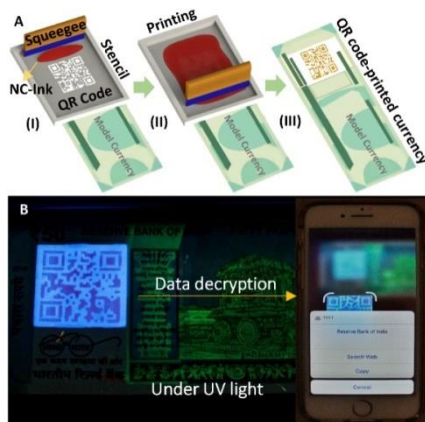


Figure 1. (A) Schematic representation of the stencil printing technique used to print QR code on a currency. (B) Data decryption processing using a smartphone under UV light.

Herein, we report the room temperature fabrication of a stable, flexible, nontoxic, and low-cost precision nanocluster-based luminescent ink for the stencil printing of an optically unclonable security label. Nanocluster-based printing inks show brilliant photoluminescence owing to its extended C–H \cdots $\pi/\pi\cdots\pi$ interactions. Spectroscopic and microscopic investigations show that intercalated nanoclusters in the printed security labels are highly stable as their optical features and molecular compositions are unaffected. The exceptional mechanical, thermal, photo, and aqueous stabilities of the printed security labels endorse to demonstrate the printing and smartphone-based electronic reading of the quick response code on a currency. Finally, confidential information protection and decryption under a precise window of light have been achieved by adopting the optical contrast illusion. The overall cost of the security label is found to be approximately 0.013 USD per stamp.⁶

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Facile Spin Coating-based Method for the Formation of Mechanoresponsive Soft Surface Wrinkles

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Abstract: Morphology of soft materials, including those of natural systems has great influence in controlling the functionality and properties of such materials. Responses of soft surfaces to external stimuli and extraneous systems are also directed by structural features of the surfaces. Natural surfaces have purpose-driven and meticulously designed morphological features suitable for specific functionalities. Artificial systems capable of emulating the morphology-dependent physicochemical responses of natural soft surfaces can be prepared through various methods. Wrinkling is an important morphological irregularity on soft surfaces which can be leveraged in this direction. Tunable and responsive nature of wrinkles on natural and artificial soft surfaces makes them an adequate tool for numerous applications in optics, adhesives, stretchable electronics, etc. The formation of soft surface wrinkles created through currently existing techniques rely on expensive chemicals, sophisticated instrumentation and complex experimental set up. Furthermore, the wrinkles produced through existing techniques are limited in terms of uniformity, tunability and stability. Here, we present a generic and simple spin coating-based method for the formation of surface wrinkle on elastomeric substrates making use of buckling instability in a bilayer system with different elasticities in each layer. A model elastomeric material, polydimethylsiloxane (PDMS) was used for demonstrating this strategy. An uncured PDMS film of different elastomer-curing agent ratio was spin coated onto a mechanically stretched PDMS film with definite elastomer-curing agent ratio. Thermal curing followed by the release of pre-strain leads to the formation of wrinkles. The wrinkles formed through this method exhibited high robustness, tunability, mechanical switchability and mechanoresponsive optical properties.

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Alkyl Chains Assisted Control over Heat-Induced Photoluminescence Switching in Divinylbenzene-Benzoxazole Derivatives

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Abstract: Organic materials exhibiting heat-induced solid-state luminescent switching are a fascinating topic of research due to their fundamental and technological relevance. However, reversible switching of solid-state fluorescence with high contrast and reproducibility is a challenging task. One promising approach towards this end is to control the mode of solid-state packing of luminescent organic chromophores with an external stimulus.¹⁻³ In the present work, we have demonstrated the alkyl chains assisted control over reversibility and range of chromism. Herein, three derivatives of 2,2'-(1E,1'E)-(2,5-bis(alkyloxy)-1,4-phenylene)bis(ethene-2,1-diyl)bis(benzo[d]oxazole) with different length of alkyl chains (C₆H₁₃:**DB-C₆**; C₁₂H₂₅:**DB-C₁₂**; C₁₈H₃₇:**DB-C₁₈**) were synthesized and their fluorescence properties were investigated in detail (Figure 1). All derivatives exhibit efficient luminescence switching in the presence of heat stimulus. Interestingly, the reversibility, range of color, and color transition temperatures are dependent on the length of alkyl chains. Our studies revealed that alkyl chains assist the self-assembly of the chromophore backbone and facilitate their reorganization in the presence of solvents. These findings reveal the structure-property relationship of thermochromic materials that would benefit the development of luminescent thermochromic solids. Details of the study will be presented.

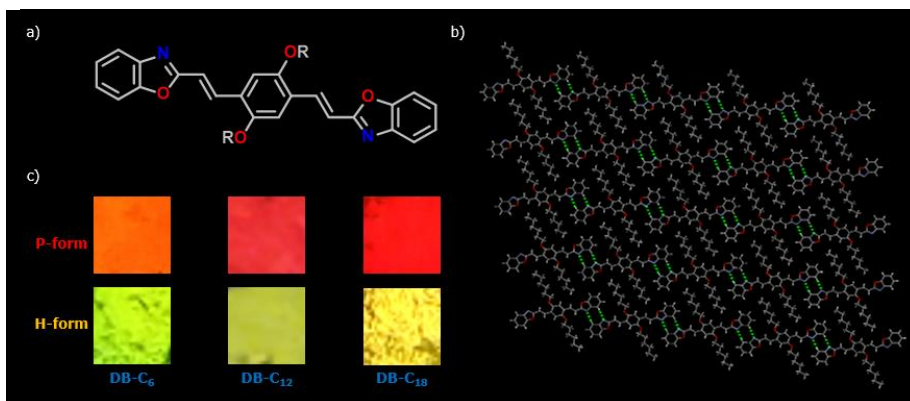


Figure 1. a) Chemical structure of **DB-C_n** b) illustration of hydrogen-bonded molecular sheet in the crystal structure of **DB-C₆** c) Photographs of the pristine and heated samples of **DB-C_n** under 365 nm UV light.

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Microwave Assisted Synthesis of S, N And C Doped ZnO Nanoparticles and Their Exceptional Photocatalytic Performance Under Solarlight Illuminations

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Abstract: The present work discusses the preparation of C, N and S doped ZnO nanoparticles through a microwave assisted polymeric gelation method. The crystallographic, optical and micro structural features of the doped ZnO nanoparticles are studied using XRD, FT-IR, UV-Visible, SEM and TEM. The efficiency of the prepared doped ZnO nanoparticles degrades an organic pollutant¹, methylene blue photo catalytically which were systematically investigated under solar light illuminations. The photocatalytic studies carried out by using UV-Visible spectrophotometer shows that both N and S doped ZnO nanoparticles² are effective in photo degrading the organic pollutant among which S doped ZnO nanoparticles has higher efficiency³ to degrade methylene blue. The order of the photocatalytic activity of doped ZnO follows the order as S-ZnO > N-ZnO > ZnO.

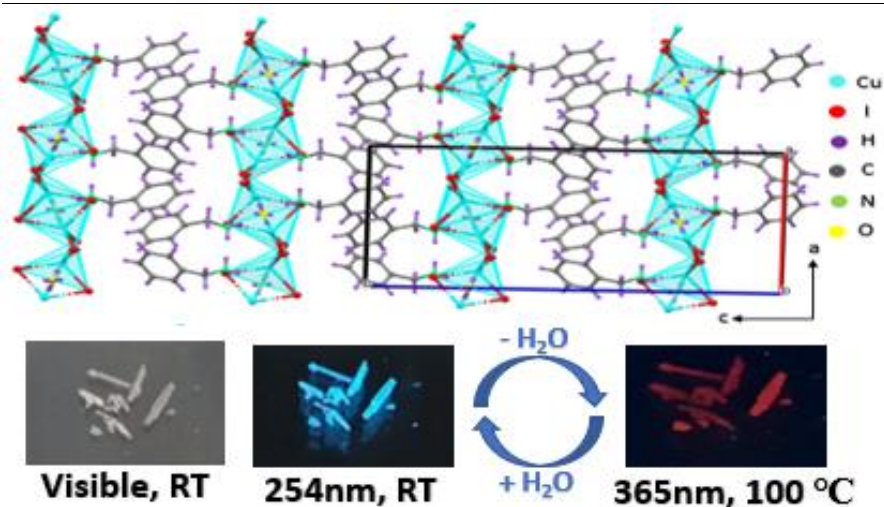
Thermally-Induced Fluorochromism in Lead-Free Hybrid Halide Single Crystals $\text{Bz}_2\text{Cu}_2\text{I}_4\cdot\text{H}_2\text{O}$

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Abstract: Organic–inorganic metal halide hybrids (OIMHs) have attracted widespread attention among the research community because of their diverse applications in photovoltaics, LEDs and lasers. Considering the toxicity of lead (Pb)-based materials, the research world sought after alternative candidates. Thus, less toxicity, earth-abundance, cost-effectiveness makes the Cu(I) halides promising for optoelectronic applications. Herein, we introduce a two-dimensional Pb-free OIMH single crystal with a formula $(\text{Bz})_2\text{Cu}_2\text{I}_4\cdot\text{H}_2\text{O}$ (Bz: benzylamine). In the crystal form, the dimeric units $[\text{Cu}_2\text{I}_4]^{2-}$ are connected through corner share and edge share in an alternative manner to form a cyclic hexagonal cage like two-dimensional array. The $(\text{Bz})_2\text{Cu}_2\text{I}_4\cdot\text{H}_2\text{O}$ single crystal exhibits a blue emission centered at 473nm, which could be originating from the self-trapped excitonic emission mechanism. The large Stokes shift of 156nm and a broad full-width half maximum (FWHM) of ~95nm are the highlights of this material. It exhibited outstanding reversible thermally-induced fluorochromism from blue to red at temperature near 100 °C.



The SCXRD structure $(\text{Bz})_2\text{Cu}_2\text{I}_4 \cdot \text{H}_2\text{O}$ SC (top). The optical images showing thermally-induced fluorescence switching.

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Some Aspects of Transition Metal Oxide Based Devices for Energy Management

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Abstract: Energy is essential to maintain and increase the standard of living. Energy saving are becoming more urgent because of its increasing demand day by day due to rising population. The use of energy is mostly dwelt with various sectors like industry, transport and in buildings especially it is utilized for heating, cooling, lighting and ventilation. As people spend their most of the time in indoor environment related to their carriers which tend to spend as much as energy for space cooling. One way to improve the situation with regard to energy and indoor comfort is to have building envelopes with variable throughput of visible light and solar energy. In line with these worldwide efforts, use of smart windows will significantly decrease the cost of air conditioning and sun shading, and simultaneously improve the indoor comfort with added decoration effect [1]. Such windows are mostly relying on the chromogenic technologies in which the optical properties can be changed in response to external signal. Chromogenic materials based on transition metal oxide (TMOs) can alter their optical properties via the application of some external stimuli like potential, temperature, light etc [2]. Herein we demonstrated a facile, low cost, environment friendly technique to synthesis photochromic solution of WO_3 -PVP, V_2O_5 -PVP composite. These solutions show good photochromic behavior under the irradiation of UV light 365nm with coloring time of 3s and bleaching time of 30mins with good kinetics. The major challenge in this solution is to make bleaching time lesser. This property of the composite in altering the optical properties pave the way for real time applications like smart displays, smart windows, glasses, optical memory devices, security systems.

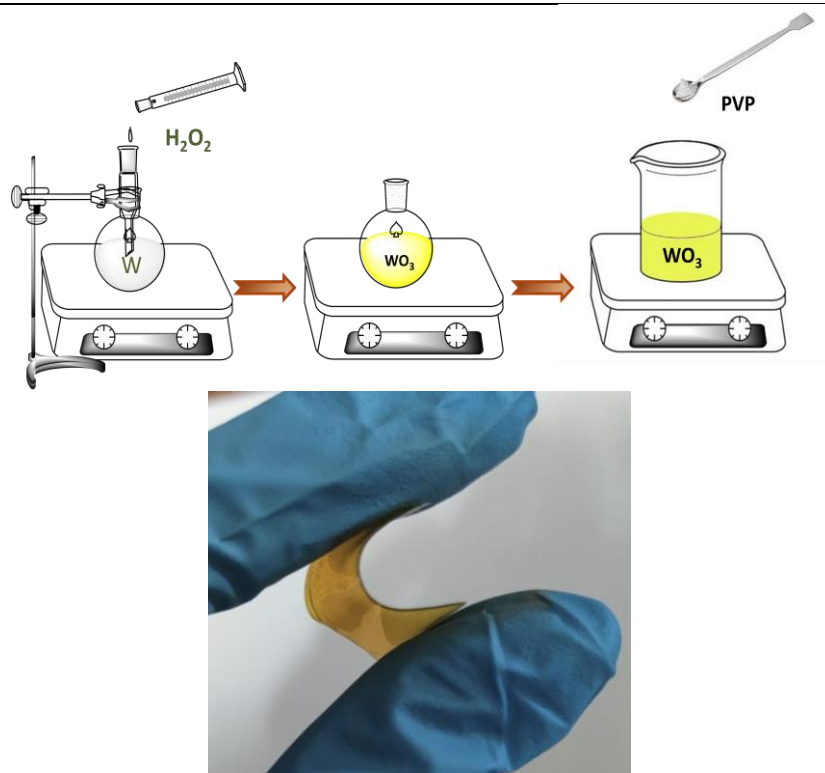


Fig.1. A. Experimental setup B. Result-Flexible photochromic film

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Synthesis and Thermal Characterization of Chitosan Derivative

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Abstract: The work is focused on the synthesis of a green and renewable polyelectrolyte complex (PEC) containing phosphorous, nitrogen and carbon, with an aim to analyze the kinetic behavior and propose different methods to study the degradation kinetics of the fabricated material. The preparation of PEC was based on the ionic complexation between an innocuous acid named phytic acid (PA) and a biopolymer called chitosan (CS). The FTIR and thermal characteristics of the same were studied. Kinetic parameters under non-isothermal condition were calculated using FWO, KAS, Starink and Tang model free methods. The Fourier transform infrared spectroscopy confirmed the ionic complexation between positively charged CS and negatively charged PA indicated by the presence of new absorption bands at 1540 cm^{-1} and 1067 cm^{-1} . An increase in the overall thermal stability for PEC was also observed with a parallelism trend in the plots which indicated a similar kinetic behavior and can be attributed to a similar reaction mechanism. Thus a water-soluble PEC consisting of bio-resourced phytic acid and chitosan was fabricated. Also the activation energy values obtained by both the methods coincide indicating the suitability of the methods to study the degradation kinetics of the materials.

Keywords: FWO, KAS, Starink, Tang, Thermal modeling

Sustained Urea Release by Preparation of Composites of Urea with CO₂-Philes Using Supercritical CO₂ as Solvent

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Abstract: Over the years, many novel and innovative industrial strategies using liquid and supercritical CO₂ solvent system have emerged by virtue of the inherent capabilities of this solvent system such as ease of solvent removal and tunability of solvent parameters. In spite of its limitations in terms of understanding its full solvent capabilities, it has made inroads into several important areas such as fluoropolymer synthesis, dry cleaning, chemical separations and processing, pharmaceutical industry, textiles industry, microelectronic cleaning, extraction of natural products and synthetic organic chemistry.

In this work we are attempting to bring together the CO₂- solvent platform and the inexpensive CO₂-philes for industrial applications considering the high solubility of these compounds. Here we introduce a novel and significant strategy for the controlled release of urea in scCO₂ medium by preparing composites of UR with CO₂-philes namely SOA and AGLU. Composites prepared were compared with those prepared in ethyl acetate medium. X-ray Diffraction (XRD) and Fourier-Transform Raman (FT-Raman) studies were carried out to study the structural and vibrational changes of the composites. Optical and Field Emission Scanning Electron microscopic (FE-SEM) studies of the composites were performed to study the morphological changes. Finally, release studies were done with the aid of Ultra-Violet Visible (UV-Vis) spectrophotometer. Effect of concentration on the release kinetics was also investigated. Finally, the two coating materials were mixed at different weight ratios and release kinetics from these composites prepared by the combination of coating materials were also studied.

Electrochemically Robust Ferberite (FeWO_4) Nanostructure as an Anode Material for Alkaline Water- and Alcohol-Oxidation

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Abstract: Iron is one of the Earth's most abundant metals and its promising catalytic performance makes it an essential nonnoble metal for energy studies. Due to the inferior conductivity and lability to dissolution during electrocatalysis, it resists to show superior electrocatalytic performance. However, recent studies on transition metal oxy-hydroxides depict that iron is the active site for OER. Herein, a heterobimetallic iron-tungstate nanostructure, synthesized solvothermally at moderate temperature, has been employed as an efficient anode material not only for alkaline OER and ethanol oxidation but also fabricated as non-noble metal-based anode for overall water-splitting. The presence of tungstate in the nanostructure improves the efficiency of OER as reflected in the overpotential value, 282 (± 5) mV at 10 mA cm^{-2} and Tafel slope of 54 mV dec^{-1} which is far better as compared to pure iron-oxyhydroxides as well as noble metal-based catalysts. A strong binding interaction with corner and edged shared $[\text{WO}_6]$ presumably provides robustness in the structure as well improves charge mobility which results in long-durability of the catalyst without changing its structure, facile electron conduction in the catalyst as well as along the electrode-electrolyte interface. The fair electrocatalytic activity of FeWO_4 anode further provides an advantage to construct a water electrolyzer coupled with commercially available Pt cathode giving a reduced cell potential of 1.66 V only to reach 10 mA cm^{-2} current density. This study showcases a facile approach to design stable anode relying on earth abundant metal precursors which remains a perdurable challenge till to-date.

Sulphonic Acid Functionalised Sba-15 as an Efficient Catalyst for The Synthesis of 2-Aryl Benzimidazoles

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Abstract: Mesoporous materials with ordered porous structure of high significance for a wide range of applications in medicine, opto-electronics, sensors, catalysis, etc. The key advantages of these materials include narrow pore size distributions, high surface area, biocompatibility, low toxicity and simple functionalisation strategies with organic moieties. SBA-15 is a highly stable mesoporous silica material with uniform ordered hexagonal array of pores with tunable pore diameter of 5 to 15 nm. SBA-15 can be easily functionalised with a wide range of moieties to impart specific properties. The present work is aimed to study the activity of sulphonic acid functionalised SBA-15 as an efficient green catalyst for the synthesis of 2-aryl benzimidazoles. SBA-15 was synthesised using the triblock polymer P123 as surfactant and tetraethyl orthosilicate (TEOS) as silica source. The functionalisation with sulphonic acid group was obtained by post grafting method using 3-mercaptopropyltrimethoxysilane (MPTMS) and subsequent oxidation of the incorporated thiol group with H₂O₂. The synthesised catalysts were characterized by FTIR, SEM, TEM, TGA and BET. The catalytic activity for the synthesis of 2-aryl benzimidazoles was screened and quantitative yield of the product was determined by GC-MS analysis.

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Dielectric and DFT Analysis of a Classic Glass Forming Liquid: Trioctyl Phosphate

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Abstract: The molecular mobility of a classic glass forming liquid, trioctyl phosphate (TOP), was investigated by broadband dielectric spectroscopy (BDS) and density functional theory (DFT) calculations. On exploring the system over wide temperature and broad frequency window, structural (α -) and secondary relaxation processes (β -, γ -) were observed.^{1,2} The α -relaxation showed a non-Debye features in frequency window and a non-Arrhenius temperature dependence, while the resolved β -relaxation showed an Arrhenius dependence. The α -process was well described by a single Vogel–Fulcher–Tammann (VFT) equation,³ glass transition temperature (T_g) was estimated to be 158.5 K and identified to be a strong glass former with a fragility index (m) of 50.2.⁴ The β -process showed an activation energy of 36.47 kJ/mol, indicating to be of intramolecular in origin from coupling model predictions.⁵ Further explorations were continued with computational calculations using Density Functional Theory (DFT) with B3LYP/6-311++G (d, p) to get molecular structural properties and other details, viz. optimized geometry, energy, dipole moment and rotational properties etc.⁶ The rotations via relaxed dihedral scans with redundant coordinates gave an activation energy of 37.5 kJ/mol for the secondary β -relaxation, which is comparable experimentally observed value of 36.5 kJ/mol from the dielectric spectroscopy and the origin of the rotations was identified to be arising from the rotations of lengthy alkyl chain and confirming that the resolved secondary relaxation is nothing but intramolecular in origin.

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Novel Organic Dye Molecules for Early Corrosion Detection

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Abstract: Early corrosion detection is a novel and demanding concept emerged in recent past. Colour assisted corrosion monitoring paves a major role in this field. In the present study, certain organic dyes were synthesized and utilised as corrosion markers by monitoring their colour changes upon complexation with metal ions. It is observed that dye molecules can form complexes with various metal ions like Fe^{2+} , Cr^{3+} showing distinct coloration and hence act as early corrosion markers. Studies have been conducted to understand the structure and complexation mechanism of dye molecules and dye molecules with metal ions.

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Assessment of Lead contamination in Soils around waste dumping sites near Calicut City

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Abstract: Heavy metal contamination has been a primary concern in urban environments. Heavy metals are more harmful than organic pollutants because they are persistent contaminants. A knowledge of the total concentration of heavy metal lead through soil analysis (as indicator) could be considered as a starting point for evaluating the degree of pollution as investigated in this study. The present study evaluated the soil contamination with heavy metal lead around two waste disposal sites located near Calicut City. Surface and subsurface soil samples from two different directions in both sites analysed for physicochemical parameters and concentration of lead. The Geo-accumulation index (Igeo) of soil samples were also calculated. The data obtained were compared with control soil samples collected from relatively undisturbed areas. From the studies it has been found that both the studied dumpsites contained heavy metal lead. In each sample investigated lead in the dumpsite soil have significant difference from those obtained in the control samples. That is, the soil around waste dumpsites had higher concentrations of lead than in the soil samples from control sites. Based on the findings, it is also found that the heavy metal concentration is generally higher at the surface than the subsurface soil. Calculated Geo-accumulation index (Igeo) shows the soil to be slightly polluted of heavy metal analysed but the C / P index place the soil as very slightly contaminated to moderately contaminated by Pb.

Highly Emissive Diphenylanthracene Based Cyano Stilbene Systems with Full Visible Range Solvatochromic Shift: A Combined Experimental and Computational Studies

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Organic fluorophores with tunable emission properties find wide potential applications such as fluorescence switches, sensors and lighting materials. The presence of strong electron donor/acceptor groups as substituents on fluorophores can commonly access strong solvatochromic fluorophore behavior through charge transfer (CT). Solvatochromism is a powerful tool for exploiting complex phenomena like intermolecular interactions and their dynamic processes, making the intermolecular interactions extremely sensitive to the small changes in the environment.

In this study, four novel diphenylanthracene based cyanostilbene derivatives with varying substituents (X = F, H, OR and NO₂) were synthesized and characterized using various spectroscopic techniques. All compounds are highly emissive, and the F substituent compound shows excellent solvatochromic behavior towards different solvents. The emission strongly depends on the solvent polarity. The optical properties of all the compounds were further assessed by density functional theory (DFT) and time-dependent DFT methods. The lower HOMO-LUMO gap of electron withdrawing substituents accounts its higher stability compared with electron donating group.

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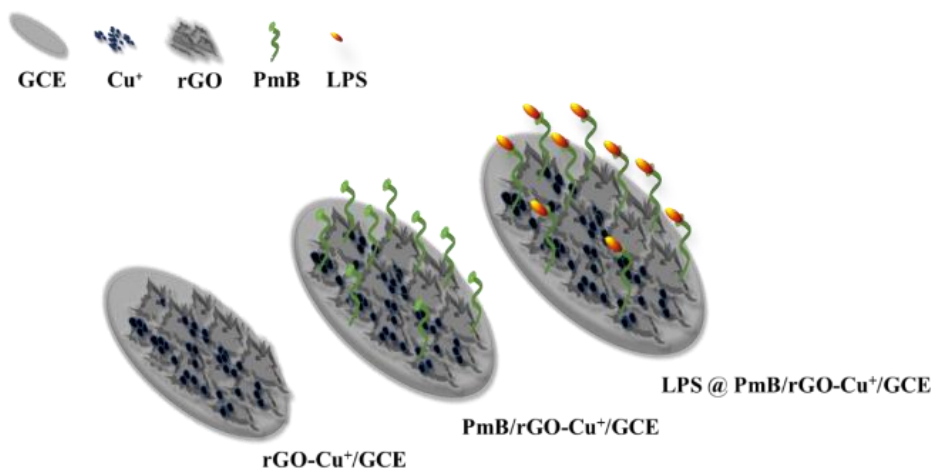
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Highly Sensitive and Selective Electrochemical Sensor for Detection of Endotoxin

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Abstract: Endotoxin or Lipopolysaccharide (LPS) is the major component of the outer membrane of gram-negative bacteria, which produces toxic effects on humans and is a major cause of septic shock and sepsis. Sepsis is a life-threatening medical emergency since it leads to tissue damage and multiple organ failure. Bacteria enter the human body through water, food products, and medical supplies and hence the detection of bacteria and bacterial toxins is of vital importance in healthcare and safety. We developed a sensitive electrochemical detection platform for the selective detection of endotoxin. We used an antibiotic immobilized, Cu⁺-reduced graphene oxide (rGO) platform as the base material for detection. The cationic antibiotic-polymyxin-B (PmB) specifically binds with the anionic groups of carbohydrate moieties of LPS leading to the selective detection of LPS plausible down to attomolar levels. The electrode exhibited an excellent response towards LPS from 10 $\mu\text{g mL}^{-1}$ to 10 ng mL^{-1} with a limit of detection of 0.32 $\mu\text{g mL}^{-1}$. The feasibility of the sensor towards practical applications in clinical studies is tested by the successful recovery of LPS from whole blood within acceptable error limits.



Schematic representation of the fabrication procedure of the PmB/GO-Cu⁺/GCE for the specific detection of LPS.

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Management of Mild Steel Corrosion in 0.5N Hydrochloric Acid Using Aqueous Leaves Extract of Garciniacambogia (GCLW) as Green Inhibitor

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Abstract: The aqueous leaves extract of Garciniacambogia(GCLW) was investigated as a green and sustainable candidate for the corrosion management of mild steel in 0.5N HCl solution. The inhibition capacity of GCLW was monitored by electrochemical methods at 303,313 and 323K, and the results are compared and contrasted by soft wares including Gaussian09, Biovia material studio, and Fukui function analysis procedure from D Mol 3 calculations. The active components of the extract were preliminary screened by IR and UV-Visible spectral techniques. The presence of higher concentration of hydroxy citric acid (HCA) in aqueous extract is found to be responsible for its increased inhibition action. 4V/V% GCLW has an efficiency of 84% at room temperature whereas efficiency decreases to 73% at 313K and to 71% at 323K. The decreases in IE with increase of temperature pin point the physical adsorption mechanism of the active components of the extract on the metal surface contrary to the results of computational methods of analysis which support chemisorption as the mode of adsorption. The chemical interaction may be originated from the donation of electron pairs from O22, H46, and H38 of Mangostine and O12 of HCA. This bond is strengthened by the back bonding of electron pairs from the filled metal orbital to C2 of Mangostine and O3 of HCA. Analysis of corrosion potential values suggest that the inhibition efficiency of the extract may developed by retarding the cathodic hydrogen evolution process and the Tafel slope analysis on the other hand recommends anodic prominence in the reaction mechanism. Hence the extract behaves as a mixed inhibitor in action. Thermodynamic adsorption suggests the Langmuir monolayer model for GCLW. The surface of the material is screened before and after the reaction at different stages to gather surface microfeatures using stereomicroscope, SEM and XPS.

Cooperative Effects of Na⁺ and Citrates on the Dissolution of Calcium Oxalate Crystals

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Abstract: Precipitation and dissolution of calcium oxalate monohydrate (CaOx) crystals are relevant due to their major role in kidney stone diseases. To such an extent, small molecules and ions can act as inhibitors to prevent the formation of calcium oxalate monohydrate crystals. Herein, we explored the role of citrate and the counter cation Na⁺ ions in the dissolution of CaO_x crystals. Citrate binds on the Ca²⁺ sites of the CaO_x crystals to form calcium citrate. Dissolution of CaO_x increases with the increase in the concentration of citrate ions and time of incubation. We observed that corrugations were formed on the surface of the CaO_x crystals after the sodium citrate treatment during the dissolution process. Theoretical studies revealed that Na⁺ occupies the vacant site of Ca²⁺ in CaO_x making a strain on the surface which leads to the subsequent deformation of the crystal.

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Supercapacitor Applications of Biogenic MnO₂ Nanoparticles and Their Composites with Poly Aniline/Activated Charcoal

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Abstract: Ternary composite of biogenic MnO₂ nanoparticles with polyaniline (PA) and activated charcoal (AC) was synthesised. The MnO₂ nanoparticles was prepared by a green route using the ethanolic extract of *Cedrus deodara* pine needles. The synthesis route involves the reduction of aqueous solution of KMnO₄. This reduction was facilitated by the phytochemicals present in the leaf extract. Polyvinyl pyrrolidone (PVP) stabilized PA was prepared by the oxidative polymerization of aniline employing ammonium persulfate as the oxidising agent in HCl. Binary composite, polyaniline/activated charcoal (PA/AC) was prepared by the polymerisation of aniline in presence of AC. The synthesised materials were characterised using different spectroscopic methods, surface screening tests, diffraction and BET studies. Electrochemical measurements carried out using different voltametric studies. The results showed that the ternary composite has a specific capacitance value of 665.4 F/g which was much higher than that of PA/AC (366.5 F/g) and PA (114.9 F/g) at 1 A/g. The prepared ternary composite has superior properties may be due to the synergistic interaction between the individual components. Thus PA/AC/MnO₂ is suitable for supercapacitor applications.

Microplastics Distribution in the Sediments of Southern Ocean

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Abstract: Southern Ocean cover approximately onesixteenth of earth's total ocean area and is made up of the portions of the world ocean south of the Pacific, Atlantic, and Indian oceans and their tributary seas surrounding Antarctica below 60° S. Microplastics are a new class of environmental pollutants have become the live issue of global concern. Sediments are the reserve of environmental contaminants such as microplastics and their analysis gives the diverse nature of the environmental chemical pattern. This study focuses on the distribution of microplastics in the sediments of Southern Ocean. Microplastics were extracted from seven sediments of Southern Ocean and further quantified. Results showed the nature of plastics as fiber, fragment and bead. Abundance on the basis of colour revealed blue, black, brown, red and yellow colours. FTIR analysis identified mainly polyethylene type of plastics in all the stations. This study serves as a baseline for the future research in the study area in terms of qualitative and quantitative aspects.

Sulfur Doped Graphitic Carbon Nitride/Porphyrin Hybrids for Photocatalytic Applications

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Abstract: Graphitic Carbon Nitride and its modified forms are transpiring as important materials for energy and sustainable applications ranging from UV-Visible light harvesting, photocatalysis, fuel cell, redox catalysts, biomedical applications, etc. The feasibility of such a broad spectrum of applications stems from the distinctive optical, electronic and chemical properties possessed by graphitic carbon nitride, in combination with facile synthesis from low-cost precursors and thermal/ chemical stability. Considerable amount of attention has been directed towards overcoming limited visible light sensitivity and rapid charge recombination of g-C₃N₄. Some of those methods involves heteroatom doping, metal loading, coupling with carbon materials, dye sensitization, etc. As a nonmetallic dopant, S seems a good choice to adjust the position of its CB and VB, changing the electronic structure, and increasing the carrier mobility¹. Sulfur doped graphitic carbon nitride was prepared from thiourea by controlled pyrolysis. To enhance the absorption edge to visible range, it is further hybridized with porphyrins (Tetracarboxyphenyl porphyrin) with highly conjugated π electron system. Sulfur doped g-C₃N₄-TCPP hybrid was synthesized by ultrasound mediated procedure. Optical and structural characterization reveal enhancement in the photocatalytic performance which was confirmed by using degradation of ciprofloxacin as model reaction.

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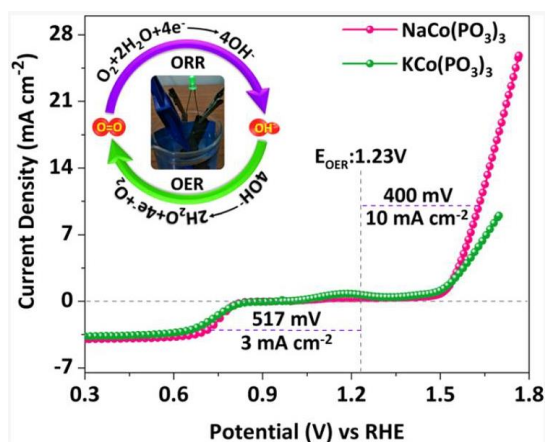
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Cobalt Metaphosphates as Economic Bi-functional Electrocatalysts for Hybrid Sodium-Air Batteries

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Abstract: Bifunctional electrocatalysts are pre-eminent to achieve high capacity, cycling stability, and high Coulombic efficiency hybrid sodium-air batteries. The current work introduces metaphosphate ($\text{Na})\text{KCo}(\text{PO}_3)_3$ nanostructures as noble metal-free bifunctional electrocatalysts suitable for the rechargeable aqueous sodium-air battery. Prepared by the scalable solution combustion method, the metaphosphate class of $(\text{Na})\text{KCo}(\text{PO}_3)_3$ with spherical morphology exhibited robust oxygen reduction as well evolution activity similar state-of-art catalysts. $(\text{Na})\text{KCo}(\text{PO}_3)_3$ metaphosphate, when employed as an air cathode in hybrid sodium-air batteries, delivered reasonably low overpotential along with excellent cycling stability with a round trip efficiency of 78%. Cobalt metaphosphates thus form a new class of bifunctional catalysts to develop hybrid sodium-air batteries



Benzodithiophene-Based Copolymer/Single-Walled Carbonnanotube Hybrids as p-Type Organic Thermoelectric Materials

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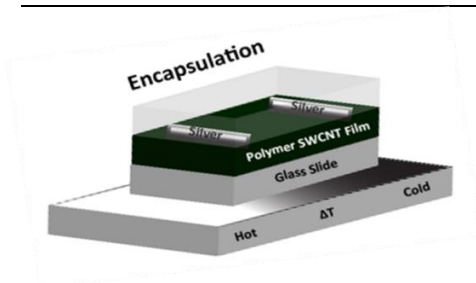
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Abstract: Conjugated polymers attracted considerable attention for thermoelectric (TE) applications. TE devices can convert waste heat into electric energy, which have been regarded as a new type of green energy source.¹ The TE performances are assessed by the dimensionless figure of merit,

$$ZT = \frac{S^2 \sigma}{\kappa} T$$

where S , σ , T , and κ are the Seebeck coefficient, electrical conductivity, temperature, and thermal conductivity, respectively. Therefore, large S , high σ , and low κ are required to obtain good TE efficiency. Organic materials usually exhibit low thermal conductivity ($<1 \text{ W m}^{-1} \text{ K}^{-1}$) that makes S and σ become the dominant components.² In this work, we prepared benzodithiophene based copolymer composite by mixing the polymer with SWCNT via probe sonication. The crystallinity of the composite was studied by XRD and the interactions between SWCNTs and polymer were examined using UV-vis-NIR absorption and Raman spectroscopy. The nanocomposite exhibited a p-type TE characteristics which increases with increasing the addition of SWCNT content. The XPS measurements were used to study the electronic structure of pristine polymer and composite film. Further, TE devices were fabricated with the as-prepared composite and silver electrode. A flexible 5 leg TE device provided an output power of 1.96 nW at $\Delta T \sim 50 \text{ K}$.



All-organic TE device

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Catalytic Degradation Studies of Methylene Blue Dye Using Cu(II) Complex Derived From 2-Hydroxy-2,2-Diphenylacetic Acid and Aminoacetic Acid

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Abstract: The Cu (II) complex have been prepared from the ligand obtained by the condensation of 2-Hydroxy-2,2-diphenylacetic acid and Aminoacetic acid. Various physicochemical and spectral measurements carried out to study and determine the structure of the complex. Degradation studies of dyes have emerged as an efficient waste water treatment method for the last few years. Plenty of studies have been still carrying out to treat the waste water flowing out from the chemical laboratories as well as textile industries. This current work focuses on the degradation study of methylene blue dye with the use Cu (II) complex obtained from the condensation of 2-Hydroxy-2,2-diphenylacetic acid and Aminoacetic acid with copper acetate solution. The catalyst prepared is found to possess high efficiency even at very small concentrations. The reaction was carried out in the normal conditions using hydrogen peroxide as oxidant and kinetics of the reaction has also been studied and order of the reaction was determined. The effect of various concentrations of oxidant and catalyst has been evaluated. The dye has been degraded (95%) in the presence of Cu (II) complex as catalyst in the minimum time period.

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Marine macroalgae *Chaetomorpha antennina* mediated green synthesis of gold nanoparticles and its catalytic efficacy in the degradation of organic pollutants

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Abstract: Biosynthesis of metal nanoparticles by means of renewable marine resources like marine macroalgae (seaweeds) has emerged as an innovative area in the current nanotechnological research. Herein, we report for the first time, the biosynthesis of well stabilized spherical gold nanoparticles (AuNPs) using aqueous extract of marine macroalgae *Chaetomorpha antennina*. The seaweed extract itself performed as the reducing agent for Au³⁺ ions and stabilizing agent for the formed AuNPs. Since no toxic chemicals involved in the synthetic strategy, it is entirely a green chemistry procedure. The biogenic AgNPs were well characterized using UV-Visible spectroscopy, High resolution Transmission electron microscopy (HR-TEM), selected area electron diffraction (SAED), Energy dispersive X-ray analysis (EDAX), X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) techniques. The outstanding catalytic activity of biosynthesized AuNPs were also evaluated spectroscopically for the hydrogenation reaction of noxious organic pollutants, Eosin yellow, methylene blue, methyl orange and Congo red by NaBH₄. Thus, the catalytically active green synthesized AuNPs may aid in the rapid elimination of industrial pollutants leading to a green environment.

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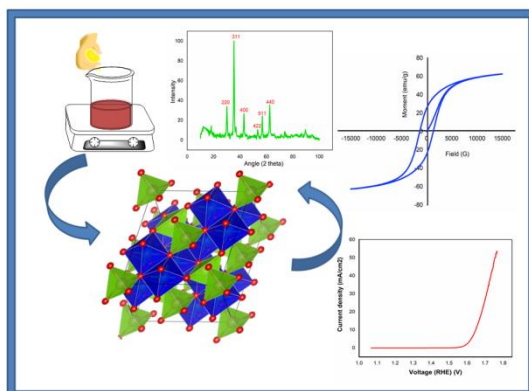
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Fabrication of Low Cost Oxygen Evolution Reaction (OER) Electro-catalyst Based on Magnetic Nanoferrite

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Abstract: The creation of an economic and efficient electro catalyst for water splitting is of prime importance to the developing renewable energy technologies. The spinel oxides of first row transition metals are widely employed for the application of OER due to their excellent stability in neutral and alkaline medium. This study reveals the magnetic properties and electrocatalytic OER activity of spinel oxide, cobalt ferrite (CoFe_2O_4) nanoparticles synthesised by a novel method (**Patent No: 360528**). An easily available lime fruit extract was used as a medium for the solgel auto combustion synthesis of cobalt ferrite nanoparticles. X-ray diffraction (XRD) studies revealed the crystallization of ferrites in cubic spinel structure. The Fourier transform infrared spectral study gives characteristic vibration bands of ferrites. XPS spectrum confirms the presence and oxidation states of Fe, Co and O elements in the samples. Vibrating Sample Magnetometer measurements (VSM) illustrate ferromagnetic nature of the sample. Saturation magnetization, magnetic remanence and the coercivity determined from the hysteresis loop are found to be in good agreement with the reported values. Under basic conditions, the nanoparticle modified electrode featured with enhanced electrocatalytic OER activity. The over potential corresponds to 10 mA cm^{-2} was found to be 410 mV versus RHE. Besides, the electrode possesses excellent stability for several OER cycles without loss of activity.



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Multi Stimuli responsive Highly AIEE Cyanostilbene Positional Isomers

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Abstract: Cyanostilbene derivatives are well known in organic optoelectronic materials such as switches, sensors and lighting devices. Here in this study, we have synthesized three cyanostilbene positional isomers with stimuli responsive emission behaviour. All the isomers are less emissive in the solution, but shows enhanced emission in the solid state. Among the three isomers the meta derivative does not shows any stimuli responsive emission, but shows highly enhanced quantum yield on grinding. The ortho isomer mechanochromic blue shift along with enhanced quantum yield. The para isomer is multi stimuli responsive and responds to different stimuli such as heat, mechanical stress and solvent vapours etc. Among the three isomers the para derivative only shows a decrease in quantum yield on grinding which may be attributed to the increased π - π stacking in the molecule. All the photophysical behaviour of the isomers are well explained using detailed single crystal X-ray studies.

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Nickel Cobaltite/Multiwalled Carbon Nanotube Modified Electrochemical Sensor for Dopamine Detection

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Dopamine plays a major role as a biomarker in both physiological diseases, addiction syndromes and drug of abuse.¹ Hence the sensitive and selective determination of dopamine is getting more attraction in the present research. Though there are a large number of reports on the detection of dopamine,² to the best of our knowledge, the real-time monitoring of dopamine, both in vitro and in vivo has not been dealt with in depth. The introduction of integrated sensors with a timely output can open the door to the mass production of miniaturized devices for the selective and sensitive detection of dopamine.³ The focus should be given to the real-time monitoring of dopamine in human samples, rather than standard dopamine solutions to prove the practicality of the sensor.⁴

Here, we report an easily synthesized nickel cobaltite/ multiwalled carbon nanotube modified sensor for the detection of dopamine. The modified sensor has a very good sensitivity and selectively detect dopamine even in the presence of a large number of interferants. The real sample analysis has been done using human neural cells, artificial sweat and serum, which further affirms the practicality of the sensor. An attempt has been made to fabricate an all-integrated flexible sensor for the detection of dopamine which is destined to become an important breakthrough in the medicinal field in the coming decade.

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Synthesis, Characterization and Antibacterial Studies of Azo Schiff's Bases of 2-(((4-ethoxyphenyl)imino)methyl)phenol

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Abstract: Schiff bases and azo compounds are important structures in the medicinal and pharmaceutical fields.^{1, 2} In light of the interesting variety of biological activities shown in compounds containing azo, alkoxy groups and azomethine linkages, it was of interest to examine the effect of having all of above functionalities present simultaneously in one structure. In this work, 2-(((4-ethoxyphenyl)imino)methyl)phenol was synthesized and novel azo dyes were prepared by reacting the Schiff base with substituted aromatic amines to form biologically active compounds. The structures of 2-(((4-ethoxyphenyl)imino)methyl)phenol, and the azo Schiff bases were confirmed by using FT-IR, ¹H-NMR, Mass, and UV-Visible spectroscopic techniques. In vitro antibacterial screening of the compounds were performed against representatives of Gram negative and gram positive bacteria by Kirby Bauer's disc diffusion method.³ Chloramphenicol was used as positive control. All the compounds showed enhanced antibacterial activity.

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A Quantitative Evaluation on the Influence of Cerium Dioxide Nanoparticles on the Growth Stages of Asian Rice Seedlings

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Abstract: Research and developments in the 21st century are mainly focused on the recent advancements in the field of Nanoscience and nanotechnology. The outburst of nanotechnology has resulted in the widespread use of industrially important nanomaterials. The release of such materials to the environment may cause important health and environmental effects. The present research interest of our group is focused on assessing the effects and impacts of globally demandable semiconducting metal oxide nanoparticles in plants. The semiconducting nanomaterials have widespread applications in the energy and environmental sectors. Among the different commercially important rare earth metal oxide nanomaterials, cerium oxide nanoparticles ($n\text{CeO}_2$) have widespread industrial applications and their interaction with the ecosystem is inexorable. The present research work is designed to explore the synergy between cerium dioxide nanoparticles and Asian rice (*Oryza sativa*) plants. This research work aims to study quantitatively the amount of cerium dioxide nanoparticles that can cause growth effects in Asian rice plants. The uptake and translocation of cerium oxide nanoparticles in Asian rice plants are also explored. The Cerium uptake, growth performance, and stress level responses in seedlings are analyzed with the help of microscopic and spectroscopic tools. Statistical analysis and characterization studies reveal that, relative to the control, $n\text{CeO}_2$ significantly reduces the growth of shoots and roots of Asia rice plants. The reasons for the reduction in plant growth are also accounted for.

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A Novel Biomimetic Approach on the Development of Artificial Antibacterial Superhydrophobic Surfaces Using Zinc Oxide Nanoparticles and Methyltrimethoxysilane (MTMS) Based Polymer Hybrids for Multifunctional Coating Applications

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Abstract: The unique combination of the surface roughness and a wax coating produces a non-wetting state on the surface of lotus leaves, allowing them to self-clean and easily shed water. Herein, we demonstrate a simple nano-technological route for producing hybrid nanoparticle metal oxide-polymer coatings on glass substrates that will biomimetic the surface of lotus leaves. The hybrid coatings were prepared through a three-tier process. Initially, a seed layer of metal oxide, ZnO, was prepared on the glass substrate by dip coating and calcination methods. After obtaining a uniform layer of seed over the substrate, the glass slides were treated in equimolar amounts of zinc nitrate and HMTA in a Teflon-lined autoclave. The unidirectionally oriented ZnO nanoparticles hence obtained on the glass substrates were further modified with Methyltrimethoxysilane (MTMS). Biomimetic, polymer - nanoparticle hybrid coatings were finally obtained. The selective uniaxial growth and crystallinity of the samples were studied by using XRD. The optical transparency of the coatings was evaluated with UV-Vis. Spectrophotometry. The functionality and structural features of the hybrid coatings were assessed using FTIR. The superhydrophobic functional characteristics of the nanoparticle-polymer-based hybrid coatings were finally evaluated by using a Contact angle analyzer. From the characterization studies and functional property assessment, the artificially prepared Metal Oxide-Polymer based hybrid coatings were found to yield good superhydrophobic properties. The present investigation can thus be advantageously utilized for developing any superhydrophobic surfaces, which can exhibit a contact angle above 150°. The antibacterial properties delivered by the glass slides were studied using the qualitative assessment method. The

present polymer-nano particle hybrid coatings find immense potential in a variety of applications in the health, defense, and industrial sectors.

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Chalcogenide Modified Titanate Perovskite: An Effective Photocatalyst

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Abstract: In the current scenario, research on energy production using semiconductor photocatalysis has grown exponentially. The main advantages of this technology includes high efficiency, environmentally benign nature and low cost. Perovskites, a class of mixed metal oxides with general formula ABO_3 , has grabbed wide attention in the field of photocatalysis due to its specific physico-chemical properties, Strontium titanate (STO) is one among the most explored perovskite system with a wide band gap of 3.2 eV. Main limitation associated with $SrTiO_3$ (STO) is its high electron-hole recombination rate and several strategies including doping, use of cocatalyst, heterojunction formation, etc. has been explored for enhancing the performance of STO.

Molybdenum disulphide (MoS_2), is a dichalcogenide with a wide range of intriguing properties, such as band-gap tunability, coupled spin and valley physics, and highly reactive edge sites for hydrogen evolution reaction (HER). As a novel semiconductor featuring a layered structure, MoS_2 is expected to improve the overall photocatalytic activity of STO by forming a heterojunction. For the present study we synthesized a $STO:MoS_2$ composite using hydrothermal method. Morphology and structural properties of the synthesized catalysts were studied using various techniques like Fourier transform infrared spectroscopy (FTIR), X-ray Diffraction (XRD) pattern, UV-vis diffuse reflectance spectroscopy (DRS) etc. Photocatalytic efficiency of the systems was scanned for the reduction of 4-nitrophenol under simulated solar radiation.

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Development of Schiff Base Furfural Phenylhydrazone as Corrosion Inhibitor for Mild Steel in 2M HCl Solution

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Abstract: Heterocyclic Schiff base furfural phenylhydrazone *FPH* was prepared and formulated as a corrosion inhibitor for mild steel in a 2M hydrochloric acid environment. Mass change measurement and electrochemical method adapted to study the effectiveness of the *FPH* during the corrosion process. *FPH* inhibitor protected 94.53 % corrosion of mild steel at optimum inhibitor strength of 0.0007 M at 303 ± 1 K. Route of corrosion protection was interpreted through adsorption of *FPH* molecules on specimen faces in acid solution. Stability of the inhibitor performance at higher temperature was studied along with various activation parameters. Mild steel corrosion protection established via Langmuir adsorption isotherm from this; thermodynamic adsorption parameters like K_{ads} and adsorption free energy (ΔG_{ads}^0) were correlated to the mild steel corrosion protection. Tafel polarization curves reveal, *FPH* molecules exhibit mixed nature inhibitors. SEM and AFM images revealed that, corroded specimen surface was severely affected by the free acid comparatively in presence of *FPH* inhibitor. The quantum chemical study revealed to explain structural and electronic structural relation to the inhibition efficiencies FT-IR analysis proved that, chemical interaction takes place between specimen surface atoms with *FPH* molecules and established coordinate type bond between them.

Electrochemical Capacitor Performance of Composite Electrodes Prepared with Polypyrrole–MultiWalled Carbon Nanotubes

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Abstract: Polypyrrole (PPy) was synthesized chemically and multi-walled carbon nanotubes (PPy/MWCNT) composites were prepared in situ. The composite material thus synthesized was well characterized by various characterization techniques. It was seen that the PPy was coated uniformly over the MWCNTs. The morphology and thickness of the coatings for various compositions were well characterized by FESEM technique. The symmetric supercapacitor cells were assembled using these composites. Highly stable cycling performance (2000 cycles without loss of specific capacitance) was achieved for the composition containing 80% PPy and 20% MWCNT in 2-electrode cell assembly at a constant current charge discharge test. The specific capacitance of the supercapacitor cell was increased to nearly 10% when the conducting additive (super-P) was added during the polymerization process than added externally to make the electrodes. The electrochemical performance of the PPy/MWCNT composite based supercapacitor cells are compositional dependent. The highest specific capacitance obtained for the cell is 184 F/g at a constant current density of 0.5 mA/cm². It is observed that even at high current density (10 mA/cm²), the cell was not experienced any IR drop indicating the usefulness of the supercapacitor cell.

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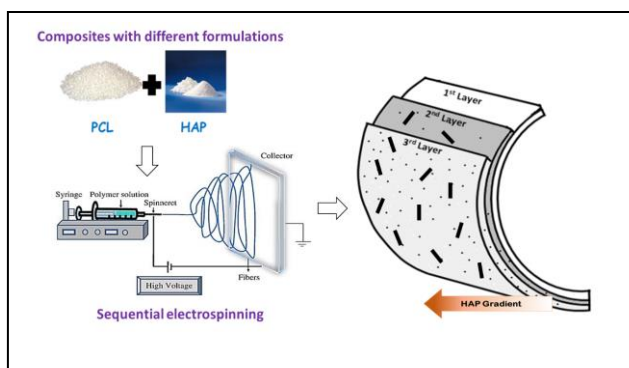
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Hierarchically Designed Electrospun Polymer Composite With Synthetic Bone Filler Towards Guided Tissue Regeneration: A Functionally Graded Approach

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Abstract: Functionally graded approach is a promising therapeutic choice for treatment of periodontal lesions. Although currently available commercial membranes function significantly in preventing the ingrowth of both gingival epithelial cells as well as connective tissues, the bioactivity and complete periodontal tissue regeneration is still an unmet challenge. The study intends to develop novel multilayered fibro porous functionally graded material (FGM) composed of polycaprolactone (PCL) with gradation in hydroxyapatite (HAP) by sequential electrospinning for guided tissue/bone regeneration (GTR/GBR) application. The tri-layered membrane with HAP gradient (0–24 w/w%) was successfully developed, composed of upper first layer with synthetic polymer PCL alone and the following PCL layers with a gradual increment of HAP concentration. Based on FGM approach, designing biomaterial with stepwise transition of bone fillers from one side of the layer to the other side across the thickness increases barrier effect and prevents delamination of layers with gradual increase in bioactivity of HAP required for bone regeneration. Morphology, thermal and mechanical properties of developed membranes were examined by scanning electron microscopy (SEM); dynamic scanning calorimetry (DSC), thermogravimetric analysis (TGA); and tensile tests (static and dynamic), respectively.



Statement of Significance: Characterization studies revealed that the graded membranes possessed enough mechanical properties and stability for clinical use. Designing hierarchical gradation of synthetic bone filler within the nanofibrous construct will be a propitious candidate for periodontal tissue regeneration.

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Revealing the Role of -OH Group on Photophysical Properties of Anthracene Substituted Salicylidenes

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Abstract: Photophysical properties of N-Salicylidene-2 amino anthracene Schiff base (2ASD) was studied on comparing with the properties of 2AAB (Benzylidene- 2 amino anthracene Schiff base) and 2AOMB (o-methoxy benzylidene – 2 amino anthracene Schiff base). Among these three molecules, the emission intensity of 2ASD is very low in the solution, while the molecule 2AAB showed a maximum emission in the solution. Absorption spectra of 2ASD were similar to the 2AAB and AOMB, and OH group do not influence the ground state property of 2ASD. However, the role of OH group on the excited state of 2ASD was understood as it undergoes ESIP, which results in the keto tautomeric form. Furthermore, fluorescence quenching is attributed to the anticipation of -OH group by providing another deactivation path. In parallel, we conducted a theoretical study that supports experimental evidence. It gives an in-depth understanding of the mechanistic aspect of keto enol tautomerism in Anthracene Salicylidene system. Here, we explored the mechanism of keto-enol tautomerism in anthracene substituted salicylidene system that may give an insight into designing molecules with desired optical properties.

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Deep Eutectic Solvent Assisted Synthesis of Dihydropyrimidinones/thiones via Biginelli Reaction

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Abstract: Deep eutectic solvents (DESs) have obtained great prominence in recent years due to their potential in the context of green chemistry. They are newly developed designer solvents, easily prepared from two or more components (one component acts as a hydrogen-bond donor and the other as a hydrogen-bond acceptor) via hydrogen bond interactions.¹ These interactions stabilize the liquid configurations and hence lower the melting temperature of the mixture.² DESs are formed by mixing the constituents with gentle heating and no additional purification step is needed. In the present work, DESs formed from hydrated metal chlorides and hydrogen bond donors (Type 4 DESs) were prepared and their catalytic activity was compared for the synthesis of dihydropyrimidinones/thiones via Biginelli reaction at room temperature. The one-pot multicomponent reaction was performed between ethyl acetoacetate, various aldehydes and urea/thiourea using DESs (Scheme 1). Among the five DESs, excellent conversion was observed using DES 2 (ZrOCl₂·8H₂O with ethylene glycol at 1:2 ratio). It may be due to the strong hydrogen bonding ability and lower viscosity of DES 2, which favors the reaction as a catalyst. The reaction was repeated using a variety of aldehydes which are used to establish the importance of this catalyst in Biginelli reaction and the products were analyzed by TLC, GCMS and NMR spectroscopy. Further, the catalyst was recycled and reused up to four consecutive cycles without significant loss in its activity.



Scheme 1 DES 2 catalyzed Biginelli reaction

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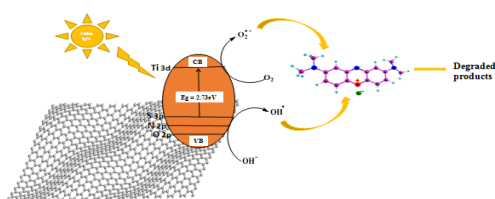
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Non-Metal Modified Nanotitania Hybridized with Graphene: An Efficient Photocatalyst

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Abstract: Graphene has two dimensional honeycomb crystal structure of sp^2 bonded carbon atoms with unique mechanical and electrical properties and offer a wide possibility to synthesis graphene-metal oxide nanocomposite for photocatalytic applications. The high specific surface area and extreme electron mobility of graphene have lead to combine the graphene with semiconductor photocatalysts for efficient photocatalytic performance.¹⁻³ Herein we designed a synthetic route to enhance the photocatalytic performance of nanotitania in the visible region by hybridizing non-metals and graphene oxide. The modified catalysts were synthesized through microwave route and were characterized by x-ray diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy (RS), and absorption studies. The photocatalytic performance of the nanocomposites towards the degradation of organic dyes under visible light was studied. Modified photocatalyst showed 98% degradation within 60 minutes.



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Electrochromic Properties of Cross-Linkable Carbazole-Diphenylamine Derivatives and Devices

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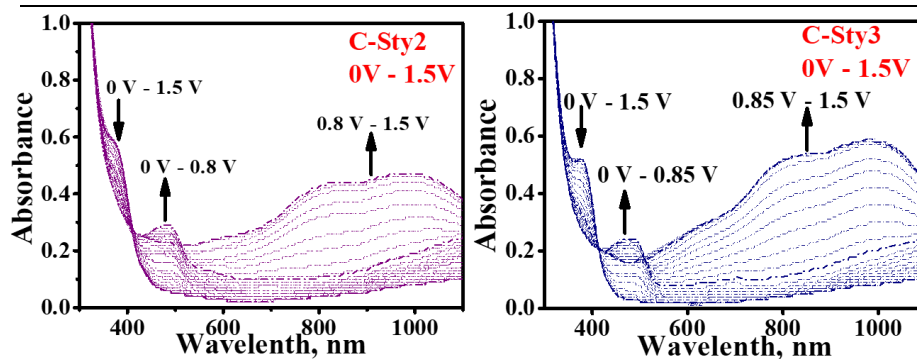
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Abstract: Electrochromic molecules and devices are able to change their transmittance, reflectance, and absorptivity due to electrochemical oxidation or reduction under an applied voltage. Electrochromic (EC) materials and devices could be utilized in displays, smart windows, electronic paper, wearable apparels and devices.¹ Triarylamine based EC materials are highly attractive and widely explored because of the easy oxidation at nitrogen center, high hole transporting ability, easy synthesis, purification, solution processability along with the option of tuning their optoelectronic properties. The stability of the film can be enhanced by introducing cross-linkable styryl moieties, which also induce better morphology and mechanical stability.² In this work, we developed two carbazole-diphenylamine derivatives (**C-Sty2** and **C-Sty3**) with thermally cross-linkable, pendant styrene groups and a model derivative (**C-OMe**) without the styrene groups and investigated their photophysical and electrochromic properties in solution, film state and EC devices. Spectroelectrochemical studies of the electrochromic films on FTO revealed multicolor electrochromism of both **C-Sty2** and **C-Sty3** (colorless–yellow–dark blue) corresponding to the radical cations and dictations formed. Fabrication of electrochromic devices using **C-Sty2** and **C-Sty3** on FTO substrates with PMMA-based solid electrolyte exhibited excellent electrochromic switching and coloration properties.



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Novel Synthesis, Characterization and Molecular Docking Studies of Dihydropyridine-2-thione

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Abstract: A number of natural compounds as well as biologically active molecules are found to possess 2-pyridone moiety as a structural unit. 2-pyridones play significant role in material science as intermolecular connectors. These compounds are usually prepared either from functionalized pyridine or by the cyclisation of acyclic systems.

Herein, we report a novel synthesis of dihydropyridine-2-thione using β -oxodithioester as synthon. The synthesis involves two steps. First step is the conversion of β -oxodithioester to thioamide using glycine ethyl ester hydrochloride in the presence of triethylamine as base in ethanol. The reaction was completed at room temperature within 4h to afford the corresponding thioamide. In the second step, the thioamide was treated with chalcone using catalytic amount of titanium tetrachloride (TiCl_4) and triethylamine as base in dichloromethane (DCM) to afford the dihydropyridine-2-thione.

The characterization was performed using IR, NMR and single crystal XRD studies. In silico molecular docking study of the synthesized compound was carried out to evaluate the anticancer activity. Molecular docking study was performed using the software auto dock and showed inhibitory property towards the proteins — human DNA topoisomerase II alpha and human DNA topoisomerase II beta. The binding energy and inhibition constant values showed that the synthesized dihydropyridine-2-thione is a promising candidate in cancer treatment.

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Comparative Green and Conventional Synthesis of 2-Hydroxy-1-Naphthaldehyde Based Barbiturates and Their DFT Study

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Abstract: 2-Hydroxy-1-naphthaldehyde based barbiturates were synthesized through an eco-friendly greener approach, by reaction of 2-hydroxynaphthalene-1-carbaldehyde with different barbituric acid derivatives in presence of natural, biodegradable, and biocompatible green catalyst chitosan-SO₃H. The use of solvent-free reaction in presence of functionalised chitosan for the synthesis of barbituric acid derivatives makes the present protocol as green and eco-friendly. A comparative study of conventional as well as solvent-free methods highlights the advantages, such as admirable yield, reduced reaction time with eviction of environmentally hazardous solvents, which leads to sustainability. Compounds were characterized by spectral techniques like IR, ¹H NMR, ¹³C NMR, and mass spectrometry. Additionally, DFT findings at M06/6-311G (d,p) level show good agreement with the experimental data which confirms the purity of entitled compounds. Natural bond orbital (NBO) analysis and non-linear optical (NLO) properties were explored at the M06/6-311G (d,p) level of theory. NBO analysis confirmed that hyper conjugative interactions are responsible for the stability of compounds. The energy gaps in compounds **5**, **6** and **7** were found as 3.822, 3.815 and 3.643 eV, respectively. Furthermore, the global reactivity parameters were calculated using FMOs energies which indicate that **5–7** hold more donating capability and stability. NLO findings confirmed that **5–7** have superior properties as compared to prototype standard compounds which unveiled their potential applications for optoelectronic technology.

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Molecular Docking Studies of Aromatic Polynuclear Schiff Base on Selected Receptors of Alzheimer's Disease

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Abstract: Alzheimer's disease (AD) is a slowly progressing neurodegenerative illness with severe social impact. The impact of AD not only related to individual but their family members and society. Patients gradually lose motor functions and cognition and in the advanced stage he/she will be unable to identify peoples. At present there are no effective pharmaceuticals or treatments that can cure AD completely. Some medicines have been developed by the scientists that can reduce the symptoms or slow down their progression of AD. Pharmaceutical scientists are in search of novel and effective drugs for AD due to their side effects of the existing drugs. The objective of the study is to evaluate the binding affinity of newly synthesized Schiff base molecule on selected receptors of AD by docking methods. In this work binding affinity of newly synthesized aromatic polynuclear Schiff bases, derived from anthrone and amino acids such as L-Arginine, L-Phenyl Alanine, L-Tryptophan respectively (A9Y5GPA, A9Y3PPA and A9Y3INPA) on selected receptors of AD is evaluated. The x-ray crystallographic structures of the receptors 1W6R and 1EVE were obtained from Protein Data Bank as pdb file. The drug likeness of the synthesized molecules was determined by Lipinski rule of five. Molecular docking and ADME prediction of the molecules were evaluated by SwissDock and SwissADME web servers. Investigations revealed that three Schiff bases bound to the 1W6R receptor protein of AD strongly than 1EVE receptor. A9Y5GPA, A9Y3PPA and A9Y3INPA showed -7.94, -7.48, and -7.84 kcal/mol binding energies respectively on the 1W6R receptor. Toxicological studies, in vitro and in vivo studies have to be conducted in future to predict the overall drugability and efficacy of these molecules to reduce the symptoms of AD.

Investigations on the Interfacial Tension Induced Self-Assembly in Tuning the 2-D Morphology of Polypyrrole at Water/Chloroform Interface

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Abstract: Self-assembly of reactive intermediates at the interface of an immiscible liquid mixture is an emerging bottom-up approach in constructing two-dimensional functional materials. Herein, we report a mechanistic investigation of the vital role of various oxidants in the self-assembly of reactive intermediates at the water/chloroform interface in pyrrole polymerization. The energetics of one-electron transfer between pyrrole and oxidant were rationalized successfully using density functional calculations. On the contrary to polymerization in single solvents, the synergistic influence of high interfacial tension and oxidant type drives the polymerization at bisolvent interface to tune the polymer morphology into two-dimensional sheets. The electron microscopic and X-ray characterization techniques confirmed the relatively uniform distribution of crystalline metal nanoparticles throughout the polymeric matrix. The electrochemical detection of potent biomarker dopamine with the limit of detection of 0.24 μM and their printability on a commercially available screen-printed electrode to detect an appreciable current indicates their potential for various electrochemical sensing applications.

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Natural Pigments in Dye Sensitized Solar Cells – Extracts from Vegetables and Fruits

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Abstract: Dye Sensitized Solar Cells (DSSCs) are emerging as one of the most promising low cost photovoltaic technologies, addressing “secure, clean and efficient solar energy conversion”.¹ A DSSC is a sandwich type solar cell comprising a photoelectrode, a counter electrode and a liquid electrolyte.² Fresh and dry extracts of natural dyes from different fruits and vegetables can be utilized³ as sensitizer in thin layer sandwich type photoelectrical DSSCs. Present work aims on prioritizing a natural pigment from different sources. Fruit extracts were taken from grapes, pomegranate, banana blossom, orange peel, red banana and dragon fruit; while vegetable extracts from spinach, carrot, beetroot and purple cabbage. Extraction technique employed was maceration.⁴ Ethanol was used as the solvent for extraction and the drying was executed using flash evaporator. Pigment characterization was carried out using FTIR and UV-Visible Spectroscopy. pH of the extracted pigments were studied, since it can predict the ample condition for adsorption of pigment onto TiO₂. The ethanol extracts did not absorb light from the visible region as the anthocyanins predominantly exist as the carbinol base form at pH values in the range of 4-6. However, in acidic solutions (pH < 2), flavylium cation predominates in the structures of anthocyanin, contributing to the red colours and is expected to exhibit absorption bands in the visible region, making it suitable for the construction of a DSSCs. Of the different sources, dyes extracted from grapes, spinach, pomegranate and beetroot was giving better yield. Dye sensitivity studies and the shelf life of pigments are to be studied.

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Effect of Schizophrenia Drugs on Dopamine Receptors to Trigger Symptoms of Parkinsonism - A Computational Evaluation

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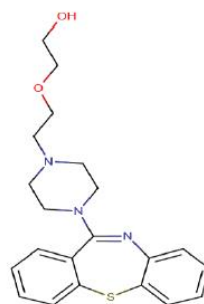
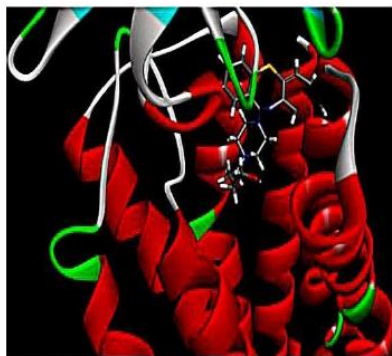
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Psychiatry is an area of medicinal science which includes the diagnosis and treatment of mental health ailment. Schizophrenia is a psychiatric disease which is characterized by thoughts that seem out of touch with reality. Patients having this abnormality show reduced participation in social activities. It affects person's ability to think, feel and behave clearly. Schizophrenia is generally treated by benzodiazepine psychiatric drugs. Benzodiazepine psychiatric drugs mainly bind with dopamine receptors D2, D3 and D4 and reduce the symptoms of Schizophrenia. Binding of these drugs on dopamine receptors cause to alleviate the production of dopamine-an important neurotransmitter in brain. This may lead to trigger the symptoms of Parkinson's disease (PD) in patients. Objective of this investigation is to study the binding capacity of selected Benzodiazepine drugs on the dopamine receptor computationally and to predict the adverse effect of the drug. Molecular docking of benzodiazepine psychiatric drugs with dopamine receptor was done using SwissDock webserver and the receptor-ligand complex was examined by USF Chimera visualizing tool. OLANZAPINE, CLOZAPINE, LOXAPINE, QUETIAPINE were the psychiatric drugs taken for the study and dopamine receptors having Protein Data bank ids 7dfp, 3pbl, 5wiu were selected for the investigation. Computational analysis showed that QUETIAPINE binds very strongly on the dopamine receptors than all other drugs. All protein-quetiapine complexes exhibited >8 kcal/mol binding energy, suggesting that this molecule is very effective psychotic drug but can enhance Parkinsonism symptoms. CLOZAPINE also showed great affinity toward the receptor 7dfp.



Keywords: *Molecular Docking, Schizophrenia, Parkinsonism*

Interaction Studies of Thiophene Substituted 1,3,4-Oxadiazole by Amines

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Abstract: The studies are on fluorescence quenching of novel thiophene substituted 1,3,4-oxadiazole derivative of 2-(4-(4-vinyl phenyl) phenyl)-5-(5-(4-vinyl phenyl)thiophen-2-yl)-1,3,4-oxadiazole (TSO) by the aromatic amine such as **o-anisidine (o-ANS)** has been studied using UV-Visible absorption, steady-state, and time-resolved fluorescence technique. Here observed that the fluorescence intensity of fluorophore TSO decreased as the concentration of **o-ANS** increased. The fluorescence quenching mechanism between TSO and **o-ANS** was analyzed using Stern-Volmer plots. The Stern-Volmer plots were found to be nonlinear with a positive deviation with an intercept equal to unity. However, the time-resolved measurements reveal that collisional interaction is involved. Estimated the different quenching parameters like Stern-Volmer constants (k_{sv}), quenching rate parameters (k_q), static quenching constant (V), and radius of the sphere of action (r) from the ground-state complex formation with sphere of action static quenching models. In addition, the magnitude of these values suggests that the sphere of action static quenching model agrees very well in our studies with the experimental results. Further, with the use of the finite sink approximation model value of k_q is greater than with the experimental value of $4\pi N^0 R^0 D$. It is suggesting that diffusion-limited reactions took place in our studies.

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Synthesis and Biological Applications of Carbon Quantum Dots Derived from Amine Modified Paper

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Abstract: We report the synthesis of carbon quantum dots (CQDs, a class of OD nanomaterials)^[1] from paper (filter paper as well as printing paper) modified with (3-Aminopropyl) triethoxysilane (APTES). The CQDs consist of a graphitic core and their shell layers are saturated by hydrogen atoms.^[2] The quantum confinement effect (QCE) in CQDs results in discrete quantized energy levels leading to a characteristic density of states (DoS) and bandgaps.^[3] The synthesized CQDs have been structurally characterized by HR-TEM, AFM, XPS, XRD, Raman, FT-IR. The optical characterizations from UV-visible and PL spectroscopy indicate the excitation-dependent emissions. CQDs synthesized here are having amine functional groups on the surface, which facilitated their usage in DNA-binding applications as well as for the development of light switches. The CQDs (filter paper and printing paper) were examined for their DNA binding, DNA cleavage and cell cytotoxicity properties.^[4] The DNA binding efficiency of CQDs in terms of their binding constants were determined and is found to be $74.015 \text{ (mg/}\mu\text{L)}^{-1}$ and $52.12 \text{ (mg/}\mu\text{L)}^{-1}$ respectively. Additionally, in order to further explore the fluorescent properties of CQD-DNA system, light switch studies were carried out^[5,6]. These studies effectuated analyzing the interaction of CQDs with CT-DNA and suggested their potential application as anticancer agents.^[7]

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