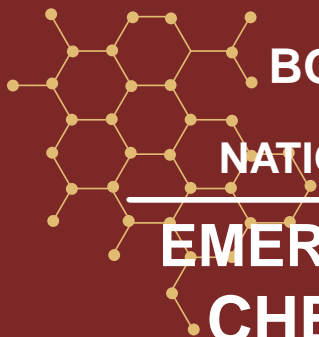


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BOOK OF ABSTRACTS
NATIONAL CONFERENCE ON
EMERGING FRONTIERS IN
CHEMICAL SCIENCES



EFCS -2020
4 – 5 DECEMBER 2020



POSTGRADUATE AND RESEARCH DEPARTMENT OF CHEMISTRY

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Preface

The Post Graduate & Research Department of Chemistry, Farook College (Autonomous), Calicut is very pleased to release the Book abstracts of the International Conference on “Emerging Frontiers in Chemical Sciences, EFCS-2020” conducted during December 04-05, 2020. This volume is an account of most of the contributions presented at the conference.

EFCS-2020 is the second national 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 National scientists and with most respected Prof. Gautam R. Desiraju, Indian Institute of Science, Bangalore, as the inaugural speaker. Another attraction is the honouring ceremony of Dr. P. S. Harikumar, Director, Water Quality Division, CWRDM by EFCS Distinguished Scientist Award for his outstanding service to Chemical Sciences and Dr. N. N. Binitha, Assistant Professor, Sree Neelakanta Government Sanskrit College, Pattambi by EFCS Young Scientist Award.

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/posters 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 organization of the conference.

December 01, 2020
EFCS 2020

Organising Committee

EMERGING FRONTIERS IN CHEMICAL SCIENCE-EFCS 2020
NATIONAL CONFERENCE
04-05 DECEMBER 2020
FAROOK COLLEGE AUTONOMOUS

Day 1, 04-December 2020 Friday

Zoom Link:

<https://us02web.zoom.us/j/83793906286?pwd=K0dFVGRyVXVlEaXlyVnVucktxRINIQT09>

- 09.15 AM- 10.05 AM : **Inaugural Ceremony**
- 10.05 AM-10.45 AM : Technical Session 1-Inaugural Talk
Prof. Gautam R. Desiraju
Indian Institute of Science, Bangalore
Topic: Role of state universities and colleges in the context of NEP2020
- 10.45 AM-11.30 AM : Technical Session 2
Prof. T. Pradeep
Indian Institute of Technology Madras
Topic: Clean water through nanotechnology
- 11.30 AM- 11.45 AM : Break
- 11.45 AM- 12.30 AM : Technical Session 3
Prof. Shobhana Narasimhan
JNCASR Bangalore
Topic: The rational design of catalysts
- 12.30 PM- 1.30 PM : **Lunch Break**
- 1.30 PM- 2.15 PM : Technical Session 4
Prof. Sameer Sapra
Indian Institute of Technology Delhi
Topic: 2D transition metal dichalcogenide nanosheets: hybrid nano-heterostructures for optoelectronic and catalytic applications

- 2.15 PM-3.00 PM : Technical Session 5
Dr. Shibdas Banerjee
Indian Institute of Science Education
and Research, Tirupati
*Topic: Ambient mass spectrometry: from
mechanistic organic chemistry to disease
diagnosis*
- 3.00 PM- 3.45 PM : Technical Session 6
Dr. T. G. Gopakumar
Indian Institute of Technology Kanpur
*Topic: Molecular materials for future
electronic devices*
- 3.45PM- 4. 15 PM : Technical Session 7
Dr. Binitha N. N.
Sree Neelakanta Government Sanskrit
College, Pattambi
*Topic: Green graphene nanocomposites for
versatile applications.*
- 4.15 PM- 5.15 PM **Paper Presentations**
Poster Presentations
(Posters will be available on the
websites www.efcs.in during
conference)

Day 2, 05-December 2020 Saturday

Zoom Link:

[https://us02web.zoom.us/j/86370982671?pwd=YUdSQUR1N2ZzOTIncEF
RNDRQSIM4UT09](https://us02web.zoom.us/j/86370982671?pwd=YUdSQUR1N2ZzOTIncEF
RNDRQSIM4UT09)

- 9.30 AM-10.15 AM : Technical Session 8
Prof. Rajakumar Balla
Indian Institute of Technology Madras
Topic: Measurement of absorption
cross-sections and kinetics of radicals
relevant to *the Earth's atmosphere using
cavity ring down spectroscopy*

- 10.15 AM-11.00 AM : Technical Session 9
Dr. Pramod P. Pillai
 Indian Institute of Science Education and Research, Pune
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Dr. G. V. Pavan Kumar
 Indian Institute of Science Education and Research, Pune
Topic: Probing single molecules with gap-plasmons
- 12.00 PM-12.45 PM : Technical Session 11
Dr. A. I. Yahya
 University of Calicut, Kozhikode
 Topic: Artificial Muscles: Materials, Technologies and Biomimetic properties
- 12.45 PM- 1.30 PM : **Lunch Break**
 1.30 PM-2.15 PM : Technical Session12
Dr. M. M. Shaijumon
 Indian Institute of Science Education and Research, Thiruvananthapuram
Topic: Batteries: beyond Lithium-ion
- 2.15 PM-3.00 PM : Technical Session 13
Prof. Satish Patil
 Indian Institute of Science, Bangalore
Topic: Exciting world of molecular electronics
- 3.00 PM-3.45 PM : Technical Session 14
Dr. Tania Francis
 St. Joseph's College, Devagiri, Kozhikode
 Topic: Biodegradable *solutions*
- 3.45 PM- 4.15 PM : **Valedictory Session**
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 Zoom Link:
<https://us02web.zoom.us/j/85062302036?pwd=bllLSTZwS0lJckJCK2RIb2lV TWpGdz09>

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Clean Water through Nanotechnology*

T. Pradeep

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Sustainable nanotechnology has made substantial contributions in providing contaminant-free water to humanity. In this talk, I present the compelling need for providing access to clean water through nanotechnology-enabled solutions and the large disparities in ensuring their implementation. I will discuss the current nanotechnology frontiers in diverse areas of the clean water space with an emphasis on applications in the field and provide suggestions for future research. Extending the vision of sustainable and affordable clean water to environment in general, I note that cities can live and breathe well by adopting such technologies. By understanding the global environmental challenges and exploring remedies from emerging nanotechnologies, sustainability in clean water can be realized. I suggest specific pointers and quantify the impact of such technologies.

*Based on our recent perspective: Clean water through nanotechnology: Needs, gaps, and fulfillment, Ankit Nagar and Thalappil Pradeep, ACS Nano, 14 (2020) 6420–6435 (DOI: 10.1021/acsnano.9b01730).

For more details, please visit: www.dstuns.iitm.ac.in/pradeep-research-group.php

The Rational Design of Catalysts

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Catalysts play a key role in modern life, in fact it has been persuasively argued that the development of the Haber-Bosch catalyst for the artificial synthesis of ammonia was the most important scientific discovery of the twentieth century. However, nearly all the catalysts in use today have been discovered either by accident, or by a process of trial and error. In recent years, efforts are underway worldwide to instead find new catalysts using an approach based on rational design. This requires a fundamental understanding of how catalysts work and what makes a material a good catalyst. This understanding can then be leveraged toward designing better catalysts for environmentally and economically important reactions such as splitting water to generate hydrogen (and oxygen).

I will give a basic introduction to the field, focusing primarily on heterogeneous catalysis, where the reactants and the catalyst are in different phases. I will discuss the important role that first principles calculations (such as those based on density functional theory) can play in helping us to understand how catalysts work, and in formulating 'descriptors' for catalytic activity. I will end by briefly presenting examples of research in my group on designing novel nanocatalysts.

Exciting World of Molecular Electronics

Satish Patil

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Research activities in our group are focused on exploring the manifold of molecular electronics ranging from organic photovoltaics, light-emitting diodes and field-effect transistors. In this seminar, I will present overview of our integrated approach of molecular design to enhance electron mobility of conjugated polymers. Specific emphasis will be placed on the guideline principle of the *donor-acceptor* approach to rationally design the low band-gap polymers and oligomers to harvest triplet excitons in organic light-emitting diodes and solar cells.

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4. Ultrafast bridge planarization in donor- π -acceptor copolymers drives intramolecular charge transfer, Palas Roy et al. **Nat. Comm.** **2017**, **8**, **1716**

Measurement of absorption cross-sections and kinetics of radicals relevant to the Earth's atmosphere using Cavity Ring Down Spectroscopy

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When a compound is released into the Earth's atmosphere, on one hand it undergoes photo dissociation when exposed to the light and on the other hand it reacts with very important oxidizing agents. Therefore, the loss of a compound depends on both photo-physical as well as photo-chemical processes, in the Earth's atmosphere. Photo induced radical chemistry plays a very important and vital role in the Earth's atmosphere in terms of Global Warming, Ozone loss and Climate change. As aliphatic as well as aromatic hydrocarbons takes the major stack in the chemical composition of the Earth's atmosphere, it is essential to understand the chemistry initiated by them in the presence of light.

Cavity Ring Down Spectroscopy (CRDS), which is essentially a supersensitive optical spectroscopic tool works on the principle of Fabry-Perrot cavity is used to measure the absorption cross-sections and kinetics with important molecules in the Earth's atmosphere. The CRD spectrometer was built in our research lab at IIT Madras. The propionyl radical, $\text{CH}_3\text{CH}_2\text{CO}$, which is of importance in both atmospheric and combustion chemistry rapidly converted to propionyl peroxy radical via its reaction with O_2 which, in turn leads to the formation of peroxypropionyl nitrate (PPN, $\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{O}_2\text{NO}_2$). PPN is an atmospheric reservoir for NO_x ($\text{NO} + \text{NO}_2$). PPN concentrations of up to 4 ppb have been measured and reported in urban areas. The visible absorption spectrum of the

propionyl radical, $\text{CH}_3\text{CH}_2\text{CO}$ was measured between 555 and 595 nm at 298 K using cross photolysis cavity ring-down spectroscopy. In addition to this, absorption cross-sections of yet few other important radicals, Phenyl radical and IO radical were measured and they were used to measure the kinetics with few important molecules^{1,2}. The details of the experimentation and results will be discussed in the conference.

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2D Transition Metal Dichalcogenide Nanosheets: Hybrid nanoheterostructures for optoelectronic and catalytic applications

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Transition metal dichalcogenide (TMD) nanosheets with defect-rich and vertically aligned edges are highly advantageous for various catalytic applications. Synthesis of TMDs using the colloidal techniques opens various possibilities to tune the electronic and optical properties of these 2D materials. As an example, we choose MoSe₂ nanosheets that have plenty of defects. The defect sites are responsible for adsorption on the surface thereby yielding excellent electrocatalytic hydrogen evolution and other catalytic activities on the surface.

Further, these defects can be employed as seeding points to grow other materials on them. Cu₂S in these defect sites leads to a Type-II semiconductor heterojunction that allows for charge separation and therefore the MoSe₂-Cu₂S forms a superior material for generation of photocurrent.

Now even heterojunctions of MoSe₂, a hexagonal crystal with CsPbBr₃ – a perovskite have been enabled by use of a linker molecule 4 – aminothiophenol. Enhanced photocurrents are obtained with such a nanoheterostructure. This methodology further opens up avenues for forming heterostructures with large lattice mismatches and can therefore be of great potential use.

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Ambient Mass Spectrometry: From Mechanistic Organic Chemistry to Disease Diagnosis

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Ambient ionization is an emerging technique for rapidly intercepting species from chemical and biological samples open to air followed by their direct analyses using a mass spectrometer. There are two components to this presentation describing our recent developments, excitements, and challenges with this technique in the area mechanistic organic chemistry and disease diagnosis. The first part of this talk will provide insight into how online ambient ionization (DESI, paper spray, electrospray, *etc.*) mass spectrometry could be used to capture transient fleeting intermediates from the reaction mixture informing details of the reaction mechanism. Our recent findings will highlight the utility of mass spectrometry for the analyses of C-H activation, elusive carbocation detection, and complex multicomponent reactions, particularly those involving short-lived, redox-reactive species, and kinetically labile transition metal salt. The second part of this talk will demonstrate the use of desorption electrospray ionization (DESI) mass spectrometry imaging technique that enables us to simultaneous visualization of the distribution of hundreds of metabolites/lipids in biologic tissues such as biopsy specimens. We employ this method of metabolic marker imaging along with heavy statics and machine learning approach for classifying cancer and benign specimens, determining cancer surgical margin, and early assessment of renal damage.

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Probing Single Molecules with Gap-Plasmons

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Confined electromagnetic fields in the gaps of plasmonic and metallo-dielectric nanostructures facilitate enhanced Raman scattering down to the single-molecule spectroscopy limit. An effective way to produce such confined 'gap-plasmonic' assisted Raman scattering is to sandwich molecules between two plasmonic or hybrid nanostructures. Alternatively, one can produce conceptually similar effect by confining molecules at the interface of colloidal plasmonic/dielectric nanostructures in a fluid and a plasmonic thin-film substrate. In recent times, confined optical fields have also been realized using self-assembled metallo-dielectric meso-structures.

We have been interested in probing gap-plasmons at metal-fluid interface [1] via , optothermal trapping, directional light scattering processes and single-molecule spectroscopic studies. In this presentation, we will discuss some insights obtained from momentum-resolved SERS from self-assembled plasmonic cavities [2]. We will highlight the emerging prospects of utilizing self-assembled metallo-dielectric architectures for fluid-phase single molecule spectroscopic studies via statistical analysis.

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Molecular Materials for Future Electronic Devices

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Thin films of semi-conducting molecules find applications in electronic devices. Due to their size, tunable electronic properties and self-assembling ability, molecules are projected as alternate building blocks for future electronic devices. In this talk I will discuss two major electronic functions of molecules on surface. a) The switching of different azobenzene (AB) derivatives on graphite surface. Using external triggers (photons and electrons), we demonstrate that the AB derivatives can be switched between two states, namely *trans* and *cis*, on surface.^{1,2} Since there is strong change in the electronic structure associated with the *trans-cis* switching, these molecules may be considered as electronic switches. b) Metal coordinated and aromatic linked molecular two-dimensional (2D) network on surface as possible electronic materials.³⁻⁵ Metal coordination and aromatic linkage enhance the electronic coupling between the molecules within the films and therefore improves the charge transport.

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Surface Ligand Directed Catalysis by Nanomaterials

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Surface ligands are ubiquitous in colloidal nanoscience. They provide the colloidal stability to nanoparticles (NPs) as well as dictate most of their physicochemical properties.^{1,2} However in the area of catalysis, the ligands have a bad reputation of poisoning the catalyst, either by hindering the surface accessibility or by creating an insulating barrier for the movement of electrons/holes.³ So, how to overcome this challenge of 'ligand poisoning'? Traditional strategies include the deposition of NPs onto a support or use ligand free NPs for catalysis. However, the available surface area and stability of NPs are often compromised during the course of catalysis. Thus, NPs and ligands are two inseparable entities, and strategies have to be developed to accomplish catalysis by retaining as well as utilizing the ligands on the NP surface. This talk will present a new strategy based on NP-reactant interaction (emanating from surface ligands) to address the challenge of '*ligand poisoning*'. By tuning the NP-reactant interaction we were not only able to achieve efficient catalysis at low NP concentration, but also to regulate the catalytic property between completely 'ON' and 'OFF' states - rendering the same NP as a catalyst or a non-catalyst.⁴ Such interaction driven enhancement in catalytic performances can be prominent in the emerging area of '*ligand directed product formation*' in NP catalysis.

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Batteries: Beyond Lithium-Ion

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Rechargeable batteries that deliver higher energy and power densities are highly essential to meet the growing energy demand from portable electronics and automotive sectors.¹ While lithium has been regarded as the future of batteries, the technology's practical limitations in terms of achievable energy densities, safety aspects, cost and availability have encouraged the scientists and manufactures to look for alternatives. The battery innovation process needs a step change in terms of breakthroughs in materials science & engineering, new electrode chemistries, new electrolytes, and new architectures, that would deliver a better battery. Several alternatives such as sodium ion batteries, sodium-sulphur batteries, and metal air batteries are being explored for their potential applications. In this talk, some of our recent efforts on the fabrication of hybrid sodium-ion capacitor devices^{2,3} and organic materials-based electrodes⁴ will be discussed and some of the key challenges will be addressed.

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Artificial Muscles: Materials, Technologies and Biomimetic properties

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For decades, emulating the structure and functionalities of natural muscles remains as a challenge to the scientific community. Their actuation involves: aqueous media, electric pulse from the brain to the muscle, liberation of calcium ions, chemical reactions (ATP hydrolysis), conformational changes along natural polymeric chains (actin and myosin) with change of volume and water exchange. This actuation involves simultaneous sensing characteristics providing the living beings with a perfect consciousness of both the characteristics of the mechanical movements and the physical interactions between the organ and its environment: muscles, nerves and brain constitutes the reference for developing intelligent system. Artificial muscles are materials/devices responding to external stimuli producing mechanical movement and having some functional similarities to biological muscles. Potential materials proposed for artificial muscles are polymers –known as Electroactive Polymers (EAP), which expand and contract when an external stimulus is applied and the technology required is multidisciplinary in nature. Progress towards achieving artificial muscles/bio artificial muscles will lead to significant benefits in biomedical area including bionic implant, cochlear implant, bio electrode, catheter steering elements, human body- machine interfacing etc. Materials, technologies and challenges with a special emphasis on conducting polymer based artificial muscles and their biomimetic sensing and actuating properties are being discussed here.

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Biodegradable Solutions

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Eco-friendly packaging - the need of the hour has become a rapidly growing area of research. In daily use packaging applications, the demand for compostable, biodegradable or recyclable packaging is high. Conventional packaging materials developed from synthetic polymers causes serious environmental issues. Recent researches are focussing on developing ecofriendly packaging materials either from biodegradable synthetic polymers or from natural biopolymers. The limitation of these materials in packaging are their poor performance due to low mechanical strength and poor barrier properties. In order to overcome this, the concept of biocomposite formation has been adopted by many researchers. The presentation aims at generating a discussion on the possibilities of polysaccharide based composites and their application in packaging. Cellulose, starch or chitosan based composites showed better mechanical strength, thermal stability, barrier properties and biodegradation rate.¹⁻³

The presented work focuses on the development of bio-composites based on high density polyethylene (HDPE) prepared by melt mixing with varying concentrations of chitosan as biofiller, maleic anhydride as compatibilizer and palm oil as plasticizer. The variation in the free volume, microstructure and crystallinity of the prepared composites has been studied using Positron annihilation lifetime spectroscopy (PALS), Dynamic mechanical analysis (DMA) and X-ray diffractometry respectively. The dielectric and thermal properties of HDPE-chitosan films has also been analyzed and compared. Coats-

Redfern model has been used to compute the activation energy of thermal degradation of the synthesized composites.

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Green Graphene Nanocomposites for Versatile Applications

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High electron mobility as well as excellent chemical and thermal stability makes graphene suitable for versatile applications. High surface area of graphene allows the well dispersion of various organic and inorganic materials over it leading to the formation of variety of nanocomposites having synergistic properties. The commercial and economic production of graphene is mainly based on graphite oxide assisted routes; but with the resultant of a graphene having additional functionalities, disturbing its π -conjugation. The corrosive chemicals and highly oxidising conditions used in graphene oxide preparation is a challenging factor on the use of graphene for biological and environmental applications. Here, a mild and green method of carbohydrate polymer assisted liquid phase exfoliation of graphite is adopted for the production of graphene dispersion. Cobalt oxide is incorporated to the graphene sheets and the electrocatalytic activity of the nanocomposite towards 4-nitrophenol (4-NP) is investigated. Further studies on the extension of the use of the cobalt oxide – graphene nanocomposite modified electrodes towards the selective and sensitive sensing of aquatic pollutant 4-NP is on the road.

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ORAL PRESENTATIONS

O1

Targeting Cancer Cells Using Cytotoxic Copper(II) Complexes Loaded Functionalized Mesoporous Silica Nanoparticle

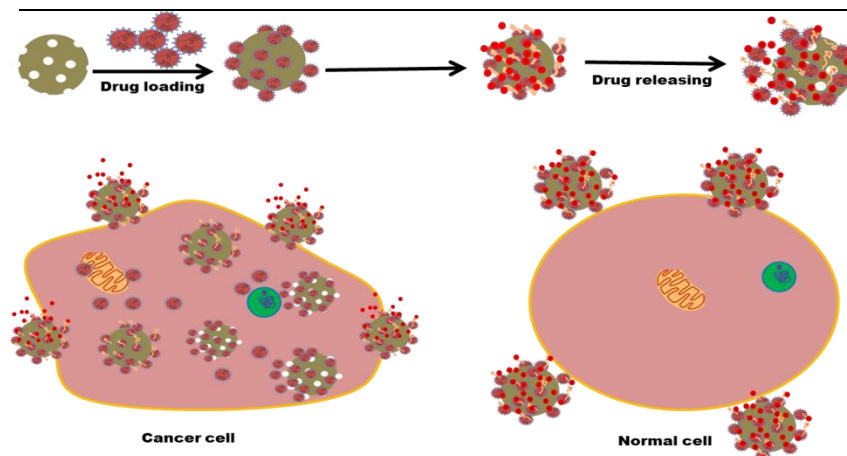
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Targeted drug delivery using nanocarriers is one of the much-explored techniques for the past one decade to eradicate the cancer disease. In recent times, many attempts have made to deliver metallodrugs at the cancer site; however, fewer reports available for copper-based cytotoxic agents. Recently, we reported a few mixed ligand copper(II) complexes of L-proline and diimine induced ROS-mediated cell death.¹ The selectivity towards the cancer cell hasn't examined for those complexes. Therefore, a drug delivery platform was constructed with cytotoxic copper(II) complexes, smart gatekeepers, and targeting agents functionalized mesoporous silica nanoparticles to deliver a loaded cytotoxic agent at the cancer site. In this regard, herein, we constructed a pH and glutathione responsive intelligent mesoporous silica nanocarriers (MSN) by incorporating cytotoxic mixed ligand copper(II) complexes in response to extracellular/ intracellular acidic environment of the tumour. After that, the attachment of folic acid/silver nanogates offers receptor-mediated endocytosis and increases selectivity towards cancer cells.



Additionally, glutathione triggered drug release achieved through the dismantling of AgNPs in the intracellular GSH environment. Free and loaded nanocarriers CC-MSN-Rh@AgNPs and CC-MSN-FA were characterized systematically by SEM, TGA & DSC, X-ray diffraction (XRD) and infrared, fluorescence spectroscopy, UV-Visible spectral techniques. In addition, cytotoxicity studies revealed that copper(II) complex (CC) loaded nanocarriers were efficiently internalized and showed better cytotoxicity against A549 cancer cells and left normal cells healthy. The above results confirmed that folate-functionalized nanoparticles successfully delivered the cytotoxic copper complexes against cancer cells, whereas healthy cells were less affected.

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Oxadiazole Based Conjugated Polymer Nanocomposites for Nonlinear Optics

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Pi-conjugated materials are of great importance in the rapidly growing field of organic electronics due to their unique features upon interaction with light. The reinforcement of such systems with compatible nanoparticles can lead to the generation of novel composite materials with enhanced optoelectronic and mechanical properties. Two nitrophenyl supported poly(1, 3, 4-oxadiazole)s viz; poly[pyridine(2-nitrophenyl)-1, 3, 4-oxadiazole] [PPNO] and poly[2-(*o*-nitrophenyl)-5-phenyl-1, 3, 4-oxadiazole] [PNPPO] were initially synthesized by a dehydrocyclization reaction, and then reinforced with TiO₂ nanoparticles. The nanocomposites have been found to possess charge transfer characteristics from the macromolecular systems (PPNO or PNPPO) to TiO₂ particles, upon photo-excitation. In view of user-friendly device fabrication, flexible films of PPNO and PNPPO were fabricated by blending the composites with 2 wt% of poly(methylmethacrylate). The nonlinear optical responses and optical limiting behaviour of PPNO, PNPPO and their nanocomposites were evaluated by Z-scan technique using nanosecond Nd:YAG, 532 nm laser radiations. They possessed strong nonlinear absorption coefficient and a nonlinear refraction coefficient of the order 10⁻¹⁰esu

and a third-order nonlinear susceptibility of the order 10^{-11} esu. The nonlinear optical properties of the matrix were found to be enhanced upon TiO₂ loading, as typically attested with the PNPPPO/TiO₂ system. Loading of TiO₂ nanoparticles onto polymer matrices has also been found to contribute to a quantum enhancement in tensile properties in the range of 20 MPa-22 MPa. These observations clearly point towards the potential use of TiO₂ loaded PNPPPO composites for use in photonic devices and optical switches, and for optical power limiting applications.

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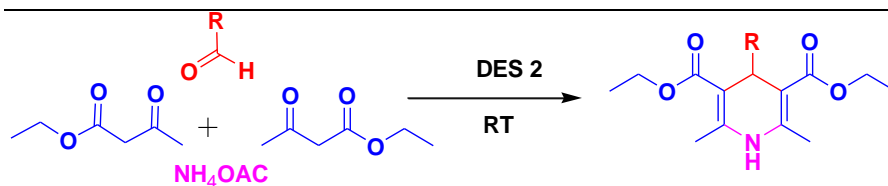
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Deep Eutectic Solvents: A Green Catalyst and Reaction Medium for the Synthesis of Dihydropyridine Derivatives

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A binary composition of two constituents, which are liquid at ambient temperature (freezing point, ≤ 25 °C) is called deep eutectic solvents, with a melting point much lower than the pure constituents.¹ The strong hydrogen bonding interaction between them makes a very large depression in their melting point compared to pure constituents.² The general mode of preparation include the mixing of two components with moderate heating and are first reported by Abbott *et al.* They are emerging green solvent and have loomed as an adorable alternative to conventional organic solvents and ionic liquids with unique properties and are non volatile, biodegradable, biocompatible, cost effective and exhibit a wide liquid range. In the present work, suitability of six DESs for the synthesis of 1,4-dihydropyridine derivatives are reported. After the completion of the reaction, the catalyst/ solvent was recovered by simple filtration, washed with minimum amount of ethyl acetate, dried and then reused in five successive reactions. The synthesized products were analysed by TLC, GCMS and NMR spectroscopy.



Scheme 1. DES 2 catalyzed Hantzsch pyridine synthesis.

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Phase Inversion Technique in the Polymer Membrane Fabrication

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Membrane technology is the leading technology which holds a significant commercial impact in several areas including water treatment, chemical, metallurgical, food industries and bioseparation areas. In 1960's Loeb and Sourirajan introduced the phase inversion technique into the membrane technology.¹ It is a versatile and simple technique which allows the formation of membrane with various morphologies for different applications. In this method, membrane formation is recognized as a phase separation process and it can be accomplished by a range of techniques such as immersion precipitation, thermal induced phase separation, vapor induced phase separation, and evaporation induced phase separation.² The final membrane morphology and performance are significantly influenced by different parameters including polymer type, concentration and experimental conditions. The method allows easy tuning of the pore type of membrane by controlling ratio of solvent outflow and nonsolvent inflow. The polymer membranes of various polymers with enhanced properties are prepared using phase inversion technique and used for various applications like ultrafiltration, microfiltration, supercapacitor separator, biomedical applications etc.^{3,4}

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Effect of Mg Doping on Thermoelectric and Optical Properties of Delafossite-Type Oxide CuCrO_2

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Thermoelectric and optical properties of copper chromium oxide, a delafossite (CuMO_2) ($M = \text{Cr, Al, Ca}$ etc.), p-type, transparent conducting oxide (TCO) has been studied. To date indium tin oxide, ITO is the best n- type TCO, which boasts a low resistivity of $\sim 10^{-4} \Omega \cdot \text{cm}$ and transmittance greater than 80%. But the hole conducting counterpart (p-type) is now replacing n- type TCO's since it is showing better transmittance. Certain p- type materials show high electrical conductance and a high Seebeck coefficient. Since Copper Chromium oxide CuCrO_2 , owns a layered structure, benefit on suppressing antiferromagnetic ordering, resulting in a high electrical conductance and a high power factor. Thus CuMO_2 has attracted much attention as the promising candidate for thermoelectric and optoelectronic applications. To improve thermoelectric performance, hole-carrier doping into CuCrO_2 has been tried by partial substitution of divalent cations for Cr^{3+} site. The single doping of divalent cations of Mg for Cr^{3+} ions was carried out to increase hole carriers. The dopants exist in the divalent state with smaller ionic radius, which could lead to a relatively higher power factor. Thus, Mg ion may be the most suitable element as dopant to improve thermoelectric properties for its stable divalent state and the smallest corresponding ionic radius in all the dopants. Here CuCr-MgO_2 , were synthesised by taking equal proportion of CuO_2 , Cr_2O_3 and MgO in different weight percentages via high temperature solid-state reaction. UV studies of

post ground Mg doped CuCrO_2 powder showed increased band width. CuCrO_2 : Mg pellets of 3mm thickness and 12mm diameter were made for thermoelectric studies. Electrical conductivity, Seebeck coefficient were measured and power factor $P = \sigma S^2$ was calculated. Doped samples showed higher power factor than pristine CuCrO_2 . By varying doping percentage considerable changes in conductivity has been made and increased optical band gap were demonstrated

Synthesis, Characterization and Sensing Application of Naphthaldehyde Based Dithiosemicarbazone

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A new thiosemicarbazone based Schiff base, 2-hydroxy naphthaldehyde para phenylene diisothiosemicabazone (NPDTSc) was synthesized by the condensation of pphenylene diisothiosemicabazide with 2-hydroxy naphthaldehyde. NPDTSc was characterized by elemental analysis and modern spectroscopic methods. The chemosensing response of the receptor, NPDTSc towards lanthanide metal ions such as La^{3+} , Ce^{3+} , Pr^{3+} , Nd^{3+} , Sm^{3+} , Eu^{3+} , Gd^{3+} , Tb^{3+} , Dy^{3+} , Ho^{3+} , Er^{3+} , Tm^{3+} , Yb^{3+} and Lu^{3+} were examined in DMSO solution. NPDTSc showed a sensing response toward Ce^{3+} , Eu^{3+} and Yb^{3+} . Job's plot analysis reveals that NPDTSc binds with Ce^{3+} , Eu^{3+} and Yb^{3+} in 2:1 stoichiometric ratio. The calculated association constant (K_a) for NPDTSc for Ce^{3+} , Eu^{3+} and Yb^{3+} ions are found to be $0.166 \times 10^5 \text{ M}^{-1}$, $0.244 \times 10^5 \text{ M}^{-1}$ and $0.400 \times 10^5 \text{ M}^{-1}$ respectively, which indicates the sensor NPDTSc shows binding affinity with ions in the order of $\text{Yb}^{3+} > \text{Eu}^{3+} > \text{Ce}^{3+}$. The binding constants of the receptor NPDTSc with Ce^{3+} , Eu^{3+} and Yb^{3+} ions were studied by fluorescence spectroscopic techniques and was found to be 0.014×10^5 , 0.026×10^5 and $0.038 \times 10^5 \text{ M}^{-1}$ respectively. The binding constant values attribute the strong binding of NPDTSc with Yb^{3+} than Eu^{3+} and Ce^{3+} , which is also conformed from the UV-Visible studies.

Keywords: Chemosensing, DMSO, fluorescence spectroscopic techniques.

POSTER PRESENTATIONS

Phytochemical Mediated Greener Synthesis of Silver/Poly(1-Naphthylamine) Nanocomposites and Their Catalytic Applications Towards Reductive Degradation of Organic Pollutants

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In this study, a highly monodispersed, exceptionally stable, spherical silver nanoparticles (AgNPs) having excellent catalytic and electrochemical response was successfully synthesized by adopting microwave (MW) assisted rapid and cost-effective method using the aqueous extract of clammy cherry (*Cordia Obliqua willd*) as the green reductant for silver ion. The competent reducing and passivating potential of phytochemicals present in the clammy cherry extract have been established using UV-Visible and TEM studies which confirmed that average size of AgNPs formed was of below 10 nm. We successfully applied this green method to incorporate AgNPs in the conjugated matrix of poly(1-naphthylamine) (PNA). The synthesized AgNPs, pristine PNA and their nanocomposites have been characterized by different spectroscopic, microscopic and electrochemical techniques. The study revealed that the catalytic and electrocatalytic properties of the composites were significantly improved on incorporation metallic AgNPs. The synthesized nanocomposites were successfully employed as a heterogeneous catalyst for the reduction of 4-nitrophenol (4-NP) and methylene blue (MB) and from the apparent rate constant

calculated for the catalytic reactions, a direct correlation between the amount silver incorporated and catalytic efficacy was established.

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A Density Functional Theory Investigation on the Mechanism of Copper-Catalyzed Sonogashira Coupling Reaction using *trans*-1, 2 Diaminocyclohexane Ligand

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Sonogashira coupling reactions are considered to be one of the most widely employed transition metal- catalyzed coupling reactions for the synthesis of carbon-carbon bonds. These reactions, which involve the formation of aryl acetylenes, are deemed to be versatile tools for the fabrication of molecules having biological and pharmaceutical importance. In this presentation, we discuss a detailed computational quantum chemical study of the Sonogashira coupling reaction between aryl halides and terminal alkynes catalyzed by Copper (I) species with *trans*-1, 2-diaminocyclohexane as ligand. All calculations discussed in this presentation are performed at the Density Functional Theory (DFT) level, using the hybrid Becke3LYP functional .Our study provides the first theoretical insight into the mechanism of copper catalyzed Sonogashira coupling employing the ligand *trans*-1, 2-diaminocyclohexane. We have identified that the active catalyst species is a neutral 3-coordinate *trans*-1,2diaminocyclohexane ligated Cu (I) alkyne complex. The proposed mechanism proceeds through a concerted oxidative addition- reductive elimination pathway which involves a single transition state. This is owing to the ease of reductive elimination involving the coupling of Csp²-Csp carbon atoms and the less stable Cu (III) intermediate. This shows the mechanism of copper

catalyzed Sonogashira coupling reactions are quite different from those catalyzed by palladium. To gain further insights into the mechanism, substrates containing various functional groups are considered in our study. This work shows the relevance of a combined theoretical and experimental approach for rationally improving the cross-coupling reaction mechanisms.

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Synthesis and Characterisation of Mo Doped Cobalt Ferrite and Nickel Ferrite nanoparticles

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Magnetic nanoparticles like cobalt ferrites have gained much attention due to their wide range of applications in catalysis, energy storage and biomedical fields. Their electrical and magnetic properties can be tuned through ionic doping. In this work, pristine and Mo doped cobalt ferrite and nickel ferrite nanoparticles were synthesized by a facile citric acid assisted sol-gel auto combustion method using metal nitrates as precursors^{1,2}. The samples were characterized using Fourier Transform Infrared spectroscopy (FT-IR), Scanning Electron Microscopy (SEM) and Thermogravimetric/DSC analysis. The IR spectral analysis confirms the Mo incorporation in the metal ferrite. The scanning electron microscopic images revealed the particle sizes as ranging from 19 to 36 nm. The TG and DSC analysis showed excellent thermal stability of the material.

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‘Go green with biopolymer composites – Synthesis of Starch Chitosan blend film & a study on it’s mechanical properties’

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Polymeric materials have played a crucial role in the global industry over the past two decades. Their adaptability, durability, and cost effectiveness account for it’s extensive usage. However, many of the synthetic polymers are derived from non-renewable resources which make them incompatible with the growing environment concerns. An alternative would be introducing biopolymers such as starch, chitosan, gelatin among others which could possibly replace synthetic polymers to address and resolve these problems. This study describes the merits of composite film from two biomaterials- starch and chitosan synthesized by solution casting process with glycerol as a plasticizer. The development of these composite materials have huge scope and potential, a main feature being its biodegradability and improved mechanical properties. Pure and blend films of biopolymers could be considered for packaging, medical, and other applications. Chitosan is a pollutant in the coastal areas but possess intrinsic antimicrobial activity and film forming properties. Forming miscible composite film with hydrophilic biopolymers like starch can overcome the water resistance of pure chitosan film. The characterization of pure as well as blend films is performed by the IR studies. The influence of different ratio of starch to chitosan in the blends on mechanical properties of films are investigated, measuring the tensile strength which is an important factor to decide upon its future in food applications. This project intends to give an overview

on the importance of biopolymers in nanotechnology-based applications.



Different compositions of starch - chitosan solutions poured onto the glass trays.

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Fe(III)-mediated Photodegradation of Atrazine and Cyanuric Acid: A Product Analysis Study

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Triazine derivatives are among the most widely used herbicides and its main mode of action as herbicide is the disruption of the light reaction of photosynthesis. Contamination of ground and surface water by triazines is a serious problem in many parts of the world due to their continual use as herbicides. Triazines are stable compounds and are almost inert to direct photodegradation because of their very weak absorption of sunlight. Advanced Oxidation Processes (AOPs) are found to be more efficient for the degradation of these triazines. AOPs involve the generation of hydroxyl radical (OH), a powerful oxidizing agent, which reacts with most of the organic compounds at diffusion-controlled rate. In the present work, we have investigated the photodegradations of 6-chloro N-ethyl N'-(1-methylethyl)-1,3,5-triazine, 2,4 diamine (atrazine, AT) and cyanuric acid (CA) by the photolysis of aqueous ferric perchlorate using sunlight and UV-light at low pH. The hydroxyl radical (OH) generated from the photoreaction of the complex $\text{Fe}(\text{OH})^{2+}$, is likely to be the major active reagent. The degradation of these triazines was also studied using photolysis of H_2O_2 in which OH is undoubtedly the active species. More attention was given on the Fe(III)-mediated photolysis because of its advantage in absorbing the visible light and hence its potential environmental application. Comparison of these two methods demonstrates that photolysis in the presence of ferric perchlorate is more effective for the degradation of triazines. The details about the products generated as a result of Fe(III) mediated

photolysis in the case of AT and CA are investigated using LC-MS/MS Analysis. Product profile in the case of AT shows that in many products, the chloride is eliminated thereby reducing its toxicity. CA is the main oxidized product of AT which is generally known to be resistant to further oxidation. However, our study clearly demonstrated the oxidation of CA in the photolysis of ferric perchlorate. Furthermore, the product studies presented here give clear evidences that both the formation of OH as the intermediate and the excited state reaction of Fe(III)-organic complex are operative in the photolytic degradation of triazines in the presence of ferric perchlorate.

Quantitative Assessment of Substituent Effects in Nitroxide Radicals

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Topographical analysis of the molecular electrostatic potential (MESP) has been carried out to quantify the substituent effects for a variety of nitroxide radicals at the M062X/6-311++G(d,p) level of theory. The absolute minimum of molecular electrostatic potential¹ (V_{min}) at the oxygen atom of N–O of nitroxide radical can be used as a sensitive measure of substituent effects. The V_{min} value reflects the electron richness on NO moiety of organic nitroxide radicals, and thereby it can be used as a descriptor of reactivity or noncovalent interactions associated with >NO group.² The presence of heteroatoms, ring size and delocalization of π -electrons in the structural framework of nitroxide radicals significantly influence the magnitude of V_{min} values.³ The electron donating substituent (-CH₃) present on nitroxide radicals showed a higher negative V_{min} value, whereas an electron withdrawing substituent (-F) present on nitroxide radical displayed a lower negative V_{min} value as compared to their unsubstituted (-H) nitroxide radicals. Further, a linear relationship is established between the interaction energy of hydrogen bonded nitroxide radicals and V_{min} values.

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Rhizome Essential Oil Composition of *Zingiber Cernuum* and Its Antimicrobial Activity

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Zingiber cernuum belongs to family Zingiberaceae is a perennial herb, also called as Curved stem ginger. The rhizomes of *Zingiber cernuum* is steam distilled and the composition of essential oil was studied. The essential oil obtained was yellow in colour and the yield was about 0.007%. The chemical profile of the oil was obtained from their GC-MS analysis. The major components present in the oil are trans-Caryophyllene, alpha-Humulene and delta-3-Carene. The antimicrobial activity of the essential oil was studied using disc diffusion method. The essential oil was tested against four pathogenic stains of gram positive and gram negative bacteria. The essential oil of *Zingiber cernuum* show considerable antibacterial activity. The oil was found to be active against both gram positive and gram negative bacteria. The anti bacterial activity is mainly due to the major components present in the oil or due to the synergistic effect of the major and minor components.

Keywords: *Zingiber cernuum*; GC-MS; Disc-diffusion method

P8

Ethylene glycol: Urea: NH₄Cl as an Efficient Catalyst and Reaction Media for Knoevenagel Condensation Reaction.

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In recent years deep eutectic solvents have become attractive due to their interesting characteristics such as, physicochemical properties, low cost of components, easiness to prepare, low toxicity, bio renewability and biodegradability. In order to make the deep eutectic mixture more cost effective and renewable, carbohydrate was linked with deep eutectic mixture, since, carbohydrates are the most important and widespread renewable compound on earth. In this work we have used low melting mixtures comprised of carbohydrates to create reaction media for organic transformations. Low melting mixtures were employed as reaction media and catalyst for the effective synthesis of Knoevenagel products which made the reaction cost effective, safe and reduced use of organic solvents. Synthesis of different derivatives was done very effectively. Recyclability of the catalyst/solvent was also done.

Mitigation of Mild Steel Corrosion in Aggressive Acidic Environments Using Alcoholic Extract of *Crotalaria Pallida* as Green Inhibitor.

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In the current scenario, the usage of plant extracts as metallic corrosion inhibitors has been widely accepted. In this background the present study focuses on the utility of ethanolic extract of *crotalaria pallida* as the green inhibitor for the protection of mild steel in HCl medium. The corrosion inhibition studies were done using the gold standard gravimetric method, electrochemical impedancespectroscopy and polarization technique. Ethanolic extract of this plant leaves is rich in fatty acids along with the usual phytochemicals. The presence of these fatty acids is confirmed using various spectral and analytical techniques. The 4 v/V % ethanolic extract has 95 % inhibition efficiency in 0.5 N HCl solution at 303 K. Adsorption study of this extract indicates Langmuir unimolecular adsorption pattern of phytochemicals on mild steel surface. The mixed type surface adsorption of this extract is further supported by AFM results. Polarisation analysis again reveals the mixed type inhibition behavior of the ethanolic extract of *Crotalaria Pallida* on mild steel surface. The preliminary studies conducted at elevated temperatures throw light on the scope of its industrial and commercial application.

Synergistic Effect of CCB/MWCNT Conductive Fillers on Natural Rubber Composites

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Conductive filler reinforced Natural rubber composites have attracted immense interest among researchers owing to its prodigious potential for the fabrication of advanced materials. Extensive studies have already revealed the synergistic effects of CNT and CB in polymer composites in electrical, mechanical and in EMI shielding effectiveness.¹⁻³ In our work electrical and mechanical properties of natural rubber (NR) composite with hybrid filler system of conductive carbon black (CCB) and multi walled carbon nanotubes (MWCNT) is analyzed. The dielectric, mechanical and transport properties were studied. Frequency dependent dielectric properties are well explained through the atomic, electronic and orientation polarizations. Interphase polarizability of the CCB incorporated composites led to the increase of dielectric constant to 41.2 from 2.7 for highest filler loading compared to gum vulcanizate. Also it increases to 1801 for hybrid filler system with 1phr CNT Improvement in AC conductivity suggests the formation of continuous conductive path of CCB and MWCNT in NR matrix. Frequency dependent impedance behavior also shows the improved conductivity at higher filler loading. Higuchi, Korsemayer-Peppas and Peppas-Sahlin models were applied to transport data for better understanding of the diffusion behavior of composites. Application of Lorenz-Park and Westilinning-Wolff equations suggests improved filler-filler and filler-rubber interactions.

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Computational Investigation on the Reaction Mechanism of Charged Ozone with NO_x in the Aircraft Engine and the Atmosphere.

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The knowledge about the atmospheric chemistry has been developing day to day due to its importance in the environment and the effects related to life including health, climate and economics. Of the atmospheric particle, the mono and dioxide of nitrogen commonly called NO_x plays a key role in atmospheric chemistry. As per the international survey's NO_x are among the pollutants which cause the highest risk for human health. They also have an impact on the atmospheric physical and chemical reaction and earth radiation balance. NO_x which is an important aerosol influences the radiation budget of earth by changing the cloud scattering process. The subsonic air transport plays a major role in the atmospheric pollution due to the combustion of fossil fuel. NO_x is one of the major products of the aircraft engine fuel combustion which can be converted to the precursors of nitric acid by combining with the chemiions generated in the engines. The reaction of NO_x with O₃ is familiar but the reaction with charged ozone is unknown. In this presentation, the mechanism and thermochemistry of the reaction of NO_x with O₃⁻ which is a chemiion generated in the aircraft engine and in the atmosphere has been studied using second order Møller-Plesset second order perturbation theory and aug-ccPVTZ basis sets have also been used to calibrate the effect of the basis set functions on the optimized structures and energies of all stationary points. The structures of all reactants, products, intermediates, and transition states of reaction have been optimized and characterized. The hypersurface of potential energy surface shows only one transition point for the

reactions which confirms a direct reaction mechanism. The thermochemical analysis of the reactions shows that the barrier height for the reaction of O_3^- with NO and NO_2 is 9 kcal/mol and 29 kcal/mol respectively. Reaction pathway shows that the reaction between NO and O_3^- is an endothermic reaction and reaction between NO_2 and O_3^- is an exothermic reaction. The results obtained have important application in the broad area of physical and chemical studies of atmospheric pollutants. The new data obtained in the present study can be utilized directly for the evaluation of experiments and model predictions concerning NO_x oxidation and kinetic modelling of gas-phase chemistry of pollutants/nucleation precursors formed in aircraft engines and the Earth's atmosphere.

Keywords: *Ab initio*; atmospheric nucleation precursors; reaction of ozone anion; stratospheric reaction.

Protection of Mild Steel in Acidic Chloride Environment Using Functionalised Silica Loaded Stearic Acid Grafted Chitosan

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Mesoporous hydrophilic SiO₂ is rendered hydrophobic by using silylating agent hexamethyl disilazane (HMDS). Different weight percentages of mesoporous hydrophobic surface-modified silica were loaded into the chitosan film and further grafting with stearic acid through 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) mediated coupling reaction. The resulting chitosan-based film was characterized by FTIR, TGA, AFM, FESEM, and EDX techniques. The film formed was applied for corrosion protection of mild steel in 0.5M HCl and analysed via non-electrochemical and electrochemical techniques. EIS measurements and potentiodynamic polarization studies have proven that the chitosan-based film offers better corrosion protection to mild steel. The coating offers prolonged protection for the metal surface with enhanced hydrophobicity and barrier properties.

Plasmonic Study of Dimer Ag Nanocylinder Structure for Sensor Application

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Transmittance of silver shell nanocylinder dimer system that interact with incident plane wave is studied theoretically using 2D finite difference time domain (FDTD) method. The measure of how sensitive is the structure to the change in embedding medium paves the way of possible application in nano-sized sensor technology. Sensitivity of designed system is studied by varying controlling parameters like inter particle distance, dimension of cylinders and angular orientation of dimer system. Red shift/blue shift is observed in transmittance curve with increasing/decreasing dielectric permittivity of the medium. Intensity of transmittance as well as Sensitivity of the structure has a strong dependence on interparticle distance and radius of individual cylinder. Structure giving best sensitivity is found through multiple simulation studies which have potential application in biosensing, chemical sensing, Nano waveguides etc.

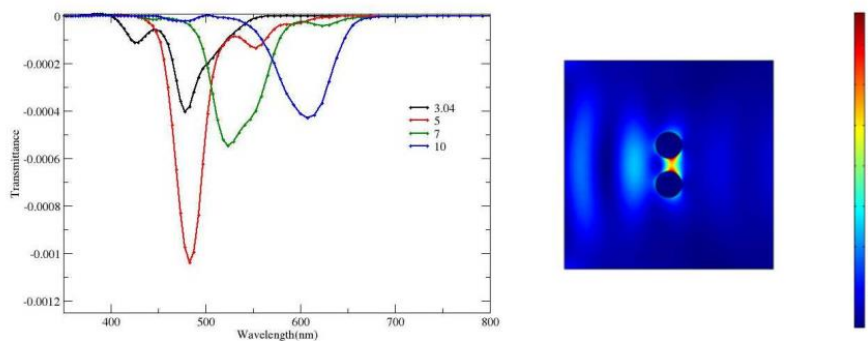


Figure 1. Transmittance characteristics as a function of wavelength for different permittivity values of sensing medium together with electric field distribution of dimer structure

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Composition of Ethyl Acetate Extract of the Bark of Strychnos-Nux-Vomica and its Antimicrobial Properties

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Strychnos-nux-vomica which belongs to the family loganiacea also called Kanjiram is a medium-sized tree. The bark of the plant was under investigation. The bark of the plant was collected and extracted using ethyl acetate solvent. GC-MS analysis was conducted to identify the components present in it. The major components present in this extract were strychnine and brucine. The antibacterial screening of the extract was carried out by disc diffusion method. The extract was tested against four pathogenic bacterial stains of gram positive and gram negative organism. The ethyl acetate extract of Strychnos-nux-vomica shows antimicrobial activity.

Key Words

Strychnos-nux-vomica, FT-IR, GC-MS, Disc diffusion method.

Kinetic and Thermodynamic Studies for Corrosion Inhibition on Mild Steel by Schiff's Base Ligand

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Schiff's base ligand L_1 and L_2 where synthesized and its inhibition action on mild steel was followed using weight loss method at 308K – 328K under 0.5M HCl. The experimental results suggest that these inhibitors are efficient to control corrosion and its efficiency increases with increase in inhibitor concentration. The energy of activation and the thermodynamic parameters were calculated and evaluated from the results of temperature studies. From this study it is revealed that the inhibition efficiency depends on both the concentration of the inhibitor and the temperature of the system. Adsorption of this compound on mild steel surface obeys Langmuir isotherm model and the ΔG^0 value suggest mixed type nature of adsorption.

Keywords: Corrosion, inhibition, temperature studies, Langmuir adsorption isotherm.

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Synthesis, Characterization and Antibacterial Screening of LLDPE doped 2-((4-ethoxyphenyl)imino)methylphenol and its Cu (II) Complex Composites.

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LLDPE (Linear low density polyethylene) is a polymer commonly used as food wraps but in most cases they are not exactly hygienic and are attacked by microbes. In this study, LLDPE doped schiff's base and schiff's base Cu (II) complex composites were prepared and made into thin sheets¹. The composites were characterized by UV-Visible and FTIR spectroscopy. The schiff's base, LLDPE/ schiff's base composites, Schiff's base Cu (II) complex and LLDPE/ schiff's base Cu (II) complex composites were subjected to in vitro antibacterial screening against gram negative *Escherichia coli* and gram positive *Staphylococcus aureus* stains at MIC of 10 mg/ml by disc diffusion method². The Cu (II) complex of the schiff's base and its polymer doped composite exhibit high antibacterial activity towards E.coli. The polymer composites can be recommended for future expansion of materials for food package, medical and pharmaceutical industries.

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Nano Dot Decorated Surface Plasmon Resonance Cavity Structure with Enhanced RI Sensing Performance

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The optics of the metal nano particles is fascinating due to the peculiar large surface to volume ratio of the particles. Noble metals with cavity in their structure can confine radiation with a greater magnitude in account of direct Surface Plasmons (SPs)-photon coupling¹. Enhanced confinement of light by extraordinary optical transmission (EOT) of light throughcavityis utilized for improve the sensitivity, were the size of cavity is tuned to get a maximum sensitivity towards refractive index of analyte. The presence of quantum dots on plasmonic cavityfurther boost the plasmon-photon coupling and thus confinement of radiation in noble metal nano structure via plasmon-exciton coupling, can be exploited for better performance of model. In this work, we propose a NDs introduced Cavity structure based on LSPR for refractive index sensing where nano dots dramatically modified the absorption/ scattering profile of the sensing platform and thus on sensing parameters together with an enhanced FOM, all confirmed by FEM stimulations.

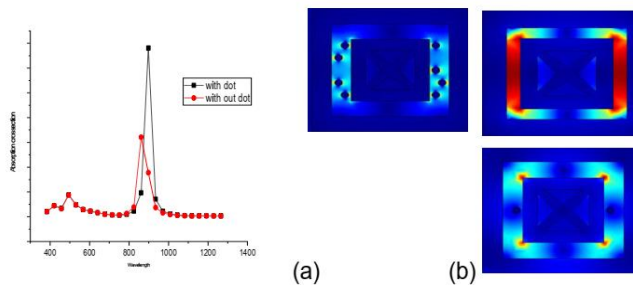


Figure.(a) Absorption cross section of cavity structure (b) 2D electric field intensity distribution .

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A Study of interaction of Anjanakallu with Eclipta Alba

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Ancient periods, highly valued medicinal plants like EcliptaAlba ,are used in Ayurvedic treatments. Eclipta Alba is also called as Bhringaraj in Ayurveda ,which has been generally utilized for a very long time as a part of conventional prescription for ailments especially related to the liver and hair .Anjanakallu or Kohl stone is other Ayurvedic product used for eye beautification and maintainence of eye from eye disorders. Anjanakallu mainly consists of Lead ,which is toxic to human body. Traditionally it is observed that, toxicity caused by Anjanakallu in human body can be cured by the application of extracts of Eclipta Alba in Ayurveda .By this concept ,a study arised based on the interaction of Anjanakallu with Eclipta Alba.

Through the studies ,it is observed that some of the components of Eclipta Alba scavenges the toxicity of lead on Anjanakallu and make it non-toxic to human body, by the formation of a complex.This observation can be strengthen using IR and UV samples of the extracts .As a result of this ,a new peak is observed in IR studies,which is similar with the peaks of the extracts used .This study intends to give an overview on the medicinal application of Eclipta Alba on Anjanakallu .

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Thiophene Based AKR1C3 Inhibitors to Target Hormone Dependent Cancers

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Aldo-keto reductase 1C3 (AKR1C3), also known as type 5 17 β -hydroxysteroid dehydrogenase (17 β -HSD). The 17 β -HSD is a NADPH dependent carbonyl reducing enzyme is involved in the metabolism of many important xenobiotic conversions. Inter-conversion of ketone and hydroxyl groups present in steroids are responsible for pre-receptor regulation and activation. AKR1C3 over expression is associated with hormone-dependent cancers such as prostate and breast cancer.¹ AKR1C3 converts the weak androgen, androstenedione into the potent androgen testosterone, and the weak estrogen estrone into the potent estrogen 17 β -estradiol. docking analysis of test compounds with AKR1C3 reveals the interaction of the test compounds Existing inhibitors of AKR1C3 having carboxylic acid functional group for better inhibitory activity.² Lot of thiophene based compounds were screened for anticancer activity in the past few years but very limited compounds reported as AKR1C3 inhibitors. Hence, in the present investigation, we designed, synthesized and characterized thiophene based compounds to target AKR1C3. The cytotoxic and apoptosis inducing potential of the test compounds were assessed by MTT and AO/EB staining respectively in MDA-MB-

231 triple negative breast cancer cells and do not show cytotoxicity. Molecular in ligand binding domain, the test compound with carboxylic acid side chain has shown better docking score (-10.285 kcal/mol) compared to the other compounds. Indomethacin was used as a positive control and it shows docking score of -11.602 kcal/mol with AKR1C3. Western blot result shows that a significant decrease in the AKR1C3 protein levels after sensitization of MDA MB-231 cells with doxorubicin before test compound treatment. Keywords: AKR1C3, estrone, androstenedione, testosterone, estradiol, molecular docking, doxorubicin, Western blotting.

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Analysis and Comparison of Water Quality Parameters of Potable and Nearby Non potable Water Resources in Feroke Municipality

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Nature has gifted us some precious and valuable resources and being one of them, water is our most basic necessities. This study focuses on the analysis and comparison of 16 physico-chemical and biological water quality parameters from 20 sources in Feroke municipality. Water samples are collected in ten sets in which one set contain a potable and non potable water resources at a particular area, the influence of the latter on the former were compared. 85% of the non potable water resources and 30% of the potable water resources exhibited acidic pH and 90% of the non potable sources exhibited biological contamination among which 65% of samples showed the presence of E.coli. One of the important facts revealed by this study is that 30% of the potable resources indicate the presence of Coliform which shows the extent of biological contamination in that region. Geographical factors are also found to influence the quality of water and the resources from swampy areas exhibited exceptionally high values for total dissolved solids and sulphate ions, samples nearby polluted lake shows the presence of undesirable components in the lake. From the survey conducted during the study, it was found that consecutive floods in 2018 and 2019 have highly influenced the quality of water bodies and about 45% of non potable resources were abandoned after the same due to increased turbidity and health effects. From the study, we conclude that it is possible to recover more

than 60% of the non potable resources and suggests that potable resources have to be disinfected before consumption.

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Computational Study on the Mechanism of Ligand Free Copper Catalyzed Suzuki Cross-Coupling Reaction using Density Functional Theory Method

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Suzuki coupling reactions are powerful tools that enable the construction of new C-C bonds efficiently, and can be employed for the preparation of diarylacetylenes, an important building block in many biologically active pharmaceuticals and natural products. Copper based catalysts are identified as a greener and cheaper alternative to traditional palladium based catalysts in cross-coupling reactions. Unlike the palladium catalyzed Suzuki coupling, copper catalyzed Suzuki coupling lacks adequate mechanistic basis. To gain deeper insights into the mechanism of the copper catalyzed coupling reactions, theoretical methods involving quantum chemistry approaches are necessary. All calculations discussed in this presentation are performed at the Density Functional Theory (DFT) level of theory. B3LYP functional was used to optimize all the structures involved in the model system, which are composed of alkynyl bromides and aryl boronic acids as the coupling partners. Our study provides the first theoretical data into the novel mechanism of ligand free copper catalyzed Suzuki coupling involving an alkynyl species. We explored the feasibility of different mechanistic pathways possible for Suzuki coupling by studying the free energy profiles for the different stages involved in the catalytic cycle for each of the

pathways. Our studies indicate that the reaction do not favour the well-established oxidative addition-transmetalation-reductive elimination pathway. Indeed, an initial transmetalation pathway is more likely to occur followed by concerted oxidative addition - reductive elimination of the coupled product. Our study could aid chemists in developing sustainable copper based catalysts for the synthesis of useful biologically active molecules like benzofuran derivatives.

Keywords: *Ligand free; Copper catalyzed; Density Functional Theory; Reaction mechanism; Suzuki coupling*

Synthesis, Characterization and Solid State Luminescence Properties of Trialkoxy Substituted Symmetric Cyanostilbene Derivatives

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Cyanostilbene derivatives have found paramount interest among various solid state emissive materials attributed to their switchable emission properties both in solid and solution states. However most of the cyanostilbene derivatives are weakly fluorescent in solution state they turn highly emissive on solid state due to a unique property known as Aggregation Induced Emission (AIE) or Aggregation Induced Enhanced Emission (AIEE).¹⁻⁴ Herein we synthesized two highly emissive alkoxy derivatives of cyanostilbene having enhanced emission in solid state and distinct solvatochromic properties. These trialkoxy substituted molecules also show liquid crystalline states similar to monoalkoxy substituted systems. The photophysical properties of the system were well studied both in liquid and solid state. The enhanced and tunable fluorescence emission behavior is the highlight of the system. The enhanced emission in the solid state may be accounted to the formation of emissive aggregate in the solid state. The vulnerability of these systems to stimuli like variation of solvent polarity is attributed to the effect of solvents on the energy levels of the molecules.

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Synthesis and Characterization of Nickel-Strontium Oxide -Citric Acid System

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Nanosize powder particles (are potentially important in ceramics, powder metallurgy, areas which require the attainment of uniform nanoporosity and similar applications. Here we describe the magnetic behaviour of Ni-Sr oxide systems on applying temperature. The nickel-strontium oxide system are prepared by the sol-gel process. The XRD analysis shows that before heating, the Ni-Sr Citric acid systems are in amorphous state and on heating at 80°C the compound changes from its amorphous state to crystalline monoclinic state. The magnetic behaviour analysis study shows that the amorphous state does not show magnetic property whereas the crystalline stated compound shows a better magnetic property. This magnetic switching property can be used in vast variety of applications.



Synthesised Ni-Sr-citric acid complex Ni-Sr-Oxide systems