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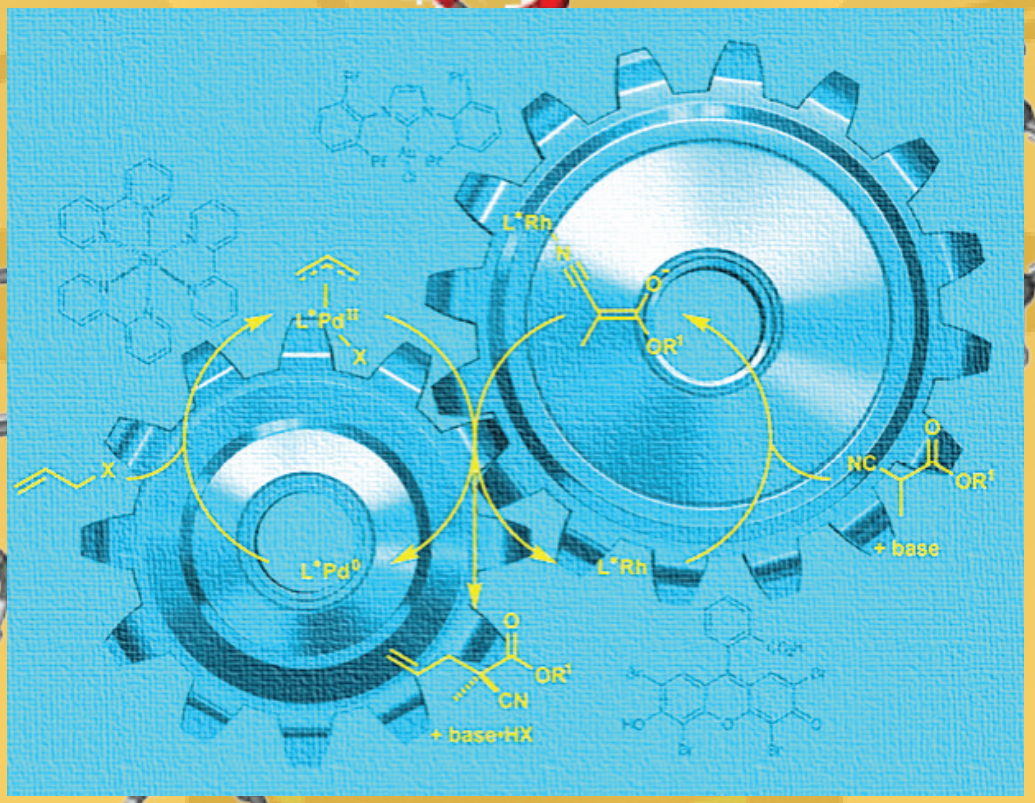
on

"Emerging Trends in Synthesis and Catalysis"

ETSC-2023

(April 12 - 13, 2023)



Organized by

Department of Chemistry
Amity Institute of Applied Sciences
Amity University Uttar Pradesh
Noida, India

Abstract Book
of
2nd International
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Message from the Chairperson

It is a great honour that Amity Institute of Applied Sciences, Amity University is organizing the "Second International Symposium on Emerging Trends in Synthesis and Catalysis (ETSC-2023)".

Synthesis and catalysis are fundamental areas of chemical research, with broad implications for a range of industries, including pharmaceuticals, materials, energy, and many more. In recent years, significant progress has been made in this field, with new methods, techniques, and materials being developed that are revolutionizing the way we think about synthesis and catalysis. Asymmetric synthesis, natural product synthesis, photochemistry and homogeneous catalysis using organometallic complexes, are some of the signature areas along with the inclusion of Artificial Intelligence and Machine Learning in synthesis and catalysis. AI is being used to design new catalysts with improved properties and selectivity. Machine learning algorithms are being applied to identify the best catalyst candidates based on vast amounts of data.

This symposium aims to showcase these exciting developments and provide a forum for the exchange of ideas and insights. We have an impressive technical programme including keynote and invited speakers, oral presentations that cover a wide range of topics, from the design and synthesis of new catalysts to the development of sustainable and green chemical processes, the symposium provides a platform for researchers, scientists, and industry professionals to come together and discuss the latest developments in the field of synthesis and catalysis.

This symposium shall also expose our faculty and students to the latest advancements in these fields and will provide an opportunity for the participants to interact and develop collaborative partnership.

I am sure that this symposium would be thought provoking and lead to germination of new ideas.

I wish the symposium a great success.

Sunita Rattan
Chairperson ETSE-2023
Dean Science & Technology
Director. Amity Institute of Applied Sciences
Amity University Uttar Pradesh, Noida

About Symposium

The prime objective of this symposium is to bring together scientists and researchers to discuss novel synthesis strategies and highly efficient heterogeneous / homogeneous catalytic methods. It presents unique opportunity for leading academicians, scientists, researchers, and scholars, to exchange their knowledge base and share their experiences and research outcomes on various aspects of green synthesis, reaction designs, catalyst synthesis & performance optimization. This two-day event will include plenary sessions, invited talks, oral and poster presentations on the most recent innovations, trends, and concerns as well as practical challenges encountered, and solutions adopted in the fields of synthesis and catalysis. We look forward to your participation in the same to make the upcoming event a memorable one for various disciplines in science.

FOCUS AREAS

- Green Synthesis
- Advanced Methods for Organic Synthesis
- Drug Design
- Polymer Synthesis: Upcoming trends
- Stereoselective Synthesis
- New materials for Sustainable Environment
- Flow Chemistry: Synthesis of Key Targets
- Bio-catalysis
- Organo-catalysis
- Catalysis for Sustainable Development
- Multiphase Catalysis
- Catalysis for Industrial Processes
- Separation Science and Process Development
- Role of Organometallic Compounds in Synthesis and Catalysis
- Computational Tools for Facilitating Synthetic Processes

Table of Contents

ABSTRACT FROM THE INVITED SPEAKERS

PLENARY LECTURE

INVITED TALKS

ORAL PRESENTATION

POSTER PRESENTATION

ABSTRACT FROM THE INVITED SPEAKERS

PLENARY LECTURE
Electrocatalysis using Nano-dimensional Materials for Green Energy and Clean Environment

Prof Pravin P Ingole

Indian Institute of Technology, Delhi

ABSTRACT

Today, the energy crisis due to depleting fossil fuel supply and their negative impact on environment like global warming is probably the world's biggest problem. Efforts have been made to develop abundant, inexpensive, and environment-friendly renewable resources of energy among which water splitting using solar light is considered as one of the most potential approaches. Moreover, the exponentially increasing global CO_2 concentration in the atmosphere has stimulated an intense research activity towards the development of economically viable technologies for environmental remediation and search for carbon-neutral energy sources. In this regard, addressing CO_2 problem on the lines of the natural photosynthetic process continues to be a major challenge for the researchers. The use of electrochemistry and nanomaterials are considered as promising avenues to address these dual challenges. In this lecture, I shall discuss few recent examples of research that have been conducted by us at IIT Delhi, India to throw the lights on the numerous applications of electrochemistry in the field of materials science and technology for the green energy and clean environmental related applications. I shall focus on the photo-electrochemical water splitting process using semiconductor materials to convert solar energy directly into chemical energy in the form of H_2 and O_2 as well as the electrochemical conversion of CO_2 and N_2 using nanostructured materials.

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INVITED TALKS
IT1:

Dually Cross-linked Gelatin-alginate Hydrogels for Tissue Engineering

Dr. Joanna Skopinska-Wisniewska

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ABSTRACT

Hydrogels are an unusual group of materials formed by cross-linking of hydrophilic polymers. They show the ability to absorb a significant amount of water and active substances, which can then be released under appropriate conditions. The high water content and elasticity make them similar to human tissues. Hydrogels with well-chosen compositions, especially natural polymers, can be an excellent environment for the life of various types of cells. The properties of the hydrogels are often modified by the cross-linking process. Both chemical bonds and physical interactions may be engaged in polymer network formation.

Dual cross-linking of a gelatin-alginate blend via ionic interactions and covalent bond creation lets us better control the shape and time of hydrogel formation as well as the properties of the final material - the mechanical resistance, porosity, swelling ability, or degradation time. Also, the biocompatibility of the materials was modulated by the selection of the appropriate cross-linking method.

The author would like to thank the National Centre for Research and Development (NCBiR, Poland, Grant no: TECHMATSTRATEG2/407770/2/NCBR/2020) for providing financial support to the project.

IT2:

Carbon-Based Catalyst for Biomass Conversion Reaction

Kushnava Bhaduri, Anirudhha Singha and Biswajit Chowdhury

Department Of Chemistry & Chemical Biology
Indian Institute of Technology (ISM)
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ABSTRACT

The need for catalyst in 21st century has been accepted by chemical community in all sectors ranging from pharmaceutical industry, fine chemicals, alternative fuels, net zero emission etc. Due to easy recovery, high turn-over, stability at higher temperature and pressure heterogeneous catalyst was proven as a superior than homogeneous catalysis. Among versatile catalyst recently carbon based composite catalyst plays an important role for waste management e,g biomass conversion. In this presentation phosphate modified carbon-silica nanocomposites were developed and characterized by several techniques for evaluating catalytic activity of glycerol esterification and glycerol carbonylation reaction. The glycerol carbonate is a bio-fuel additive which was produced substantially. The glycerol esters are fuel additives, which has the ability to strengthen the cold flow properties of the regular diesel, boost cetane number as well as cut down emission of gas. we have developed a robust and facile method for the mass production of ordered mesoporous phosphate modified carbon-silica nanocomposites via a rotary evaporation induced self-assembly method

Acknowledgement: Authors would like to IGSTC (Indo-German Centre for Science and Technology) for CO_2-Biofeed project.

IT3:

Rapid Green Analytical Methodologies for Environmental Analysis

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ABSTRACT

Prof. Kumar's research focused on the developments on green microextraction techniques using hybrid concepts of applying novel modifications in sample preparation devices or utilizing new nanomaterials that play a vital role in sample preparation because of their integral advantages over the traditional sample preparation techniques. However, these methods are multi-steps and showed poor precision/reproducibility due to a lack of semi-or fully automated processes. Therefore, our research mainly focuses on working on lab-in-syringe-based semi-or fully automated green sample preparation techniques to meet the demands of environmental analytical laboratories. In this work, novel semi-automated nanomaterials assisted green sample preparation techniques were demonstrated for the sensitive analysis of emerging environmental pollutants in environmental waters using UHPLC-MS/MS. The fabricated nanomaterials were confirmed using field-emission scanning electron microscope, transmission electron microscopy, XRD, XPS, and fourier-transformer infrared spectroscopy techniques. Various factors affecting the adsorption and desorption of emerging environmental pollutants on nanomaterials and its extraction efficiencies were studied. Under the optimal experimental conditions, maximum extraction efficiencies were achieved for all the target compounds. Applicability of the presented methods were examined with real water samples analysis. These results also proved that it is a simple, fast, efficient, low-cost, and eco-friendly method for extracting and determining toxic pollutants in environmental water samples and can be applied as a routine analytical tool in environmental monitoring and quality control laboratories. Moreover, these nanocomposites were also observed to be highly-active, low-cost, stable, eco-friendly, and efficient photo-catalyst for the complete degradation of toxic pollutants in environmental waters.

Keywords: Automation, Sample Preparation, UPLC-MS/MS, Environmental Analysis, Water Samples

IT4:

Graphitic Carbon Nitride-based Nanocomposites for the Photocatalysis of Degradation of Organic Pollutants

Suresh Sagadevan

Nanotechnology & Catalysis Research Centre, University of Malaya, Kuala Lumpur 50603, Malaysia

ABSTRACT

In recent years, a majority of people around the world are facing severe effects of environmental pollution, resulting from the rapid development of science, technology, and industries. Also, the ecological problems and energy crisis become significant challenges for human beings and so extensive research needs to be carried out to maintain sustainability. In terms of the energy crisis and related concerns, the electrical and solar devices made up of semiconductors and other photocatalysts are considered to be the most promising tools as it can be useful for the maintenance of the environment along with enhanced production of green energy. Therefore, various semiconductor photocatalysts such as graphitic carbon nitride (g-C_3N_4), TiO_2, and WO_3 have been applied widely in many fields of photocatalysis and solar devices. But the fast recombination of photogenerated carriers, the low optical absorption, and the small specific surface area is greatly limiting the performance of the above-said photocatalysts. Hence, preparing high-performance visible light catalysts remains a major challenge. The g-C_3N_4 compound has shown promising applications as an organ catalyst, photocatalyst, and highly active nitrogen source, and in addition, this material serves also as the active metal-free photocatalyst. The excellent characteristics of this material for photocatalysis include harvesting sunlight, photocatalytic stability, sufficient redox potentials to catalyze the reactions effectively, abundant and inexpensive, etc. The g-C_3N_4 was shown to be viable under visible light irradiation for both hydrogen production and organic contaminant degradation. In the present work, g-C3N4 is the most stable allotropic form of carbon nitride as it maintains a 2.7 eV optical bandgap and so it acts as an electron acceptor to extract photogenerated electrons from a metal oxide, thus increasing the efficiency of load separation within this semiconductor of oxide while limiting self-photoreduction. The present study deals with the synthesis, characterization, and photocatalytic activity of g-C_3N_4/metal oxide composite for photocatalytic applications.

Keywords: g-C_3N_4, Ternary nanocomposite, Optical band gap, Photocatalysts

IT5:

Some Aspects of Emerging Trends in Organic Synthesis

Prof. Ram Singh

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ABSTRACT

The synthesis of both simple and complex organic molecules is a requirement of all aspects of life. The development of new materials, biologically active compounds, selective transformations, new catalysts, and so on requires many sustainable efforts. The journey of synthesis started with the successful synthesis of urea in 1828. But due to the new requirements for environmental and energy concern, organic molecules synthesis is facing challenges every now and then. The journey from traditional synthesis to sustainable and green synthesis is not so easy. Organic chemists are putting a lot of effort to explore the possibilities of new methods that fulfill the current requirements of societies. Some important aspects of emerging trends will be discussed.

IT6:

“Rise of Benzoxazines: Conventional to Innovative Applications”

Dr. Bimlesh Lochab

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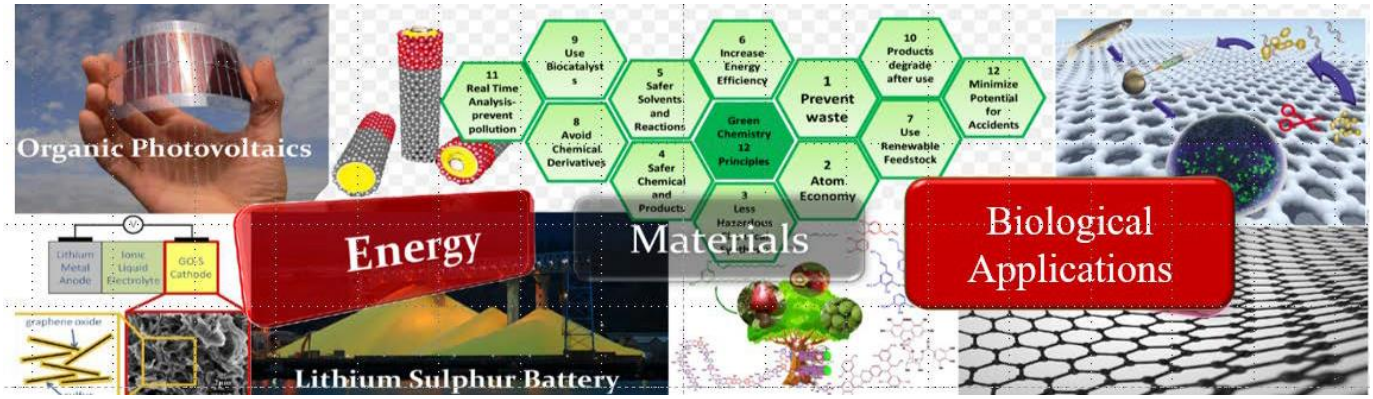
ABSTRACT

Depleting fossil fuel reserves and increasing waste reservoirs are among the world's most pressing problems. This calls for exploring naturally occurring building blocks for developing bio-based polymers. Polybenzoxazines is a new class of thermally curable thermosets being pitched as superior alternates of phenolics. In this work, we intend to exploit the options of synthesizing partially bio-based polybenzoxazines following green chemical principles of atom economy, bio-renewable feedstock, solventless synthesis, and nontoxic waste generation. In addition, the molecular flexibility of benzoxazine moiety has been utilized by studying the relation between higher functionality and properties. These polymers have shown improved thermal stability compared to their non-green counterparts and the ability to copolymerize with other industrial wastes/resources, thus finding wide applicability from adhesive and antibacterial materials to cathodes for energy storage devices.



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IT7:

Design and Strategic Synthesis of Some Biologically Important Marine Natural Products and their Fluorinated Analogues

Sunita Bhagat, Pradeep Kumar, Gunjan & Nikita Goel

Department of Chemistry ARSD College
Fellow, DSPH Institute of Eminence, University of Delhi

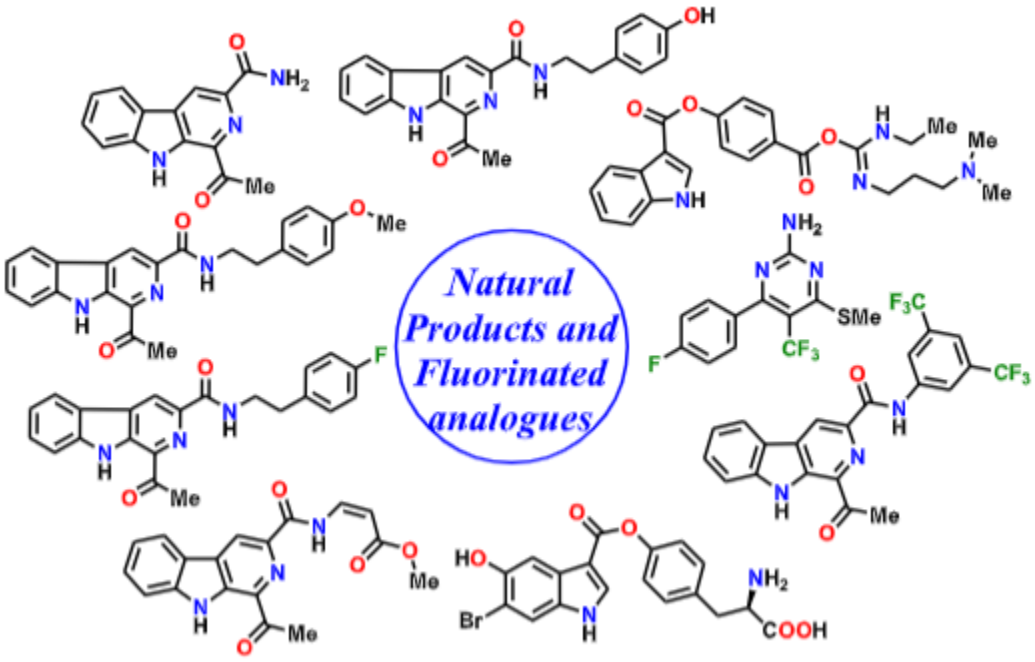
ABSTRACT

"The need for efficient and practical synthesis of biologically active molecules remains one of the greatest intellectual challenges with which chemists are faced in the 21st Century".

Throughout the ages humans have relied on Nature to cater for their basic needs, not the least of which are medicines for the treatment of a wide spectrum of diseases.[1-2] The synthesis of complex natural products continues to occupy an important position in organic chemistry research, not only because nature provides us with some of the most synthetically challenging molecules that we can ever aspire to synthesize, but also because research in this area frequently drives important breakthroughs in methodology. Structurally complex, biologically active naturally occurring substances of marine origin continue to spur the interest of both chemists and biologists as they demonstrate antiviral, antimicrobial, anti-oxidant, and many more biological activities[3-5]. Marine derived pharmaceuticals have been used as source of chemical diversity in drug discovery programmes. This was an important area to work on as the major challenge with the biologically active isolated natural products is their limited availability through natural resources and their isolation is very tedious and time consuming process[6]. Further, they are usually isolated in very small quantities, hindering further studies to establish their biological activities as well as structural modifications and their constant supply from natural sources is problematic or virtually impossible. In addition, chemoselective derivatization of marine natural products themselves is usually quite difficult because of their sensitive and elaborate molecular structures, and access to their structural analogs is severely restricted in many cases.

Therefore, chemical synthesis of marine compounds in larger quantities and by sufficient means is necessary to investigate their biological implications and this strategic synthetic methodology is focused in our lab[7-9]. We are mainly interested in natural products possessing Indole and β-carboline moieties and have extended our synthetic strategies for the synthesis of their fluorinated analogues. Synthetic utility of various functionalities such as -NH2, -COOH and -Br which are extensively used in coupling reactions has been explored in the total synthesis and which may be used in synthesizing diversely substituted analogues of many natural products and may prove helpful in establishing SAR studies. Further, considering significance of fluorine incorporation in heterocycles and taking an overview on their biological activities, synthesis of fluorinated analogues of some marine natural products is planned. An understanding of mechanism, coupled

with knowledge of physicochemical properties affected by fluorine substitution has aided in rational drug design of many pharmaceutical agents.



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IT8:

Fused/Functionalized Diazoheterocycles via metal-Catlayzed Approaches

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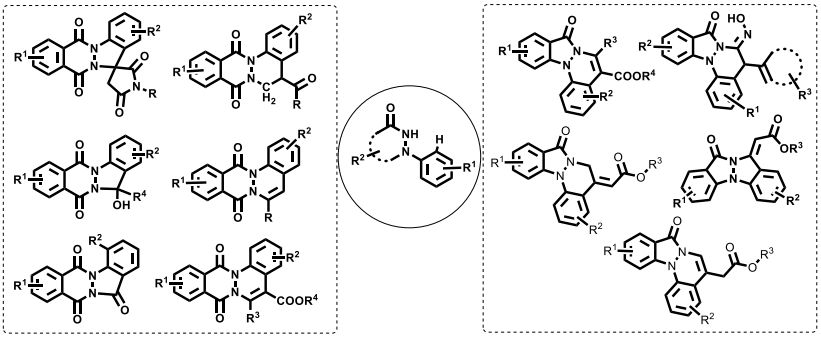
ABSTRACT

The past few decades have witnessed impressive advancements in the area of transition metal-catalyzed C-H activation strategies, exclusively contributing towards the construction of complex heterocyclic scaffolds centered on diazaheterocyclic molecular architectures. Among the known diazaheterocycles, indazole and phthalazine in their fused/functionalized forms have been recognized as valuable synthetic targets due to their wide range of applications in the field of material and medicinal chemistry. Thus, the demand of developing more efficient protocols for synthesizing fused-indazoles and fused-phthalazines in minimum number of steps from readily available precursors continues unabated. In this realm, we have successfully developed[1] eye-catching transition metal-catalyzed strategies for the synthesis of indazolo-fused indazolylidenes, hydroxy-dihydroindazolo[1,2-*b*]phthalazines, hydroxyimino functionalized indazolo[1,2-*a*]cinnolines & phthalazino[2,3-*a*]cinnolines, 6-arylphthalazino[2,3-*a*]cinnoline-8,13-diones, 5-acyl-5,6-dihydrophthalazino [2,3-*a*]cinnoline-8,13-diones, indazolo[1,2-*b*]phthalazine-triones, indazolo[1,2-*a*]cinnolines and spiro[indazolo[1,2-*b*]phthalazine-13,3'-pyrrolidine]-2′,5′,6,11-tetraones *via* directing group-assisted C-H functionalization, which shall be discussed.



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IT9:

Selecting Building Blocks for Tuning Material Properties of Protective Polyurea Coatings

Prasun Kumar Roy

Scientist 'F' Head Protective Clothing & Materials Group,
Centre for Fire, Explosive and Environment Safety, Defence Research and Development Organisation

ABSTRACT

Polyurea is a reaction product of isocyanates with s and protective coatings based on polyurea are finding extensive application in diverse fields, especially towards protection of underlying structures. Polyurea elastomers are well known for their short 'curing' times, excellent durability and exceptional adhesion to a variety of surfaces. In view of the rapid kinetics of isocyanate-amine reaction, conventional techniques like brush coating cannot be employed to form coatings. Polyurea are generally processed using spray coating process and their material properties are a manifestation of its phase segregated microstructure, which is formed of distinct ''hard'' and ''soft'' domains. For any particular isocyanate, the properties of the final product can be tailored by tweaking the constituents of the amine resin blend, especially chain extenders, chain length and crosslinker. The effect of various factors viz. soft segment length, type and concentration of chain extender and crosslinker on the material properties of polyurea are discussed.

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IT10:

Carbon Nanotube Incorporated Activated Carbon for Dye Removal from Waste Water

Shailesh Kumar Yadav and Bhanu Pratap Singh

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ABSTRACT

Water is the most basic requirement for human survival. Water contamination from dyes and coloured substances is a greater concern for safe drinking water and is difficult to remove using filtration. As a result, environmentalists and researchers are interested in the decolorization of wastewater.

Activated carbon, in the form of charcoal, has been used for purification since ancient times. However, because of their low cost, high carbon content, and widespread availability, agri-waste and biomass waste materials are the most important for the preparation of activated carbon. The removal of methylene blue (MB) and eosin yellow (EY) dyes from contaminated water were first investigated using eucalyptus bark derived activated carbon (EBAC). The time taken for dye removal by pure EBAC for MB (75%) and EY (65%) dye is ~5h.

To reduce adsorption time, a composite of activated carbon with multiwalled carbon nanotubes (MWCNTs) is prepared. The in-situ developed activated carbon has shown a synergistic effect with enhanced adsorption. In this study, adsorbent took ~60 min for the 90% removal of both dyes. In order to further reduce adsorption time and increase adsorption capacity, another composite of activated carbon with functionalized MWCNTs (F-MWCNTs) was prepared in the similar manner. The composite removes more than 90% of dye in just first 10 min at 8ppm concentration. The maximum adsorption capacity of composite for MB dye and EY dye is found as 46.43mg/g and 49.38mg/g respectively. The composite material removes dye via dual action of composite. Porous activated carbon facilitates the physisorption and functional group present on MWCNTs enhances the chemisorption of dye molecules. This composite material containing F-MWCNT is proven to be of great potential for dye removal application.

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IT11:

Role of Nanocatalysts in Biofuel Production Process

Dr G Bharath

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ABSTRACT

Biofuels production has become an increasingly important topic due to the need for sustainable and renewable energy sources. However, traditional methods of biofuels production have been found to be energy-intensive and inefficient. As a result, the use of nano catalysts has been proposed as a potential solution to enhance the efficiency of biofuels production processes. The potential of nano catalysts to improve the biofuels production process, including the conversion of biomass to biofuels and the upgrading of biofuels. A comprehensive overview of the different types of nano catalysts and their mechanisms of action in biofuels production is going to discuss. In addition, the challenges and future prospects of using nano catalysts in biofuels production processes will discuss. The use of nano catalysts in biofuels production processes has the potential to revolutionize the biofuels industry, making it more sustainable and efficient. Overall provides important insights into the potential of nano catalysts in the biofuels production process and will be of interest to researchers and industry professionals in the field.

IT12:

An Insight in to the Drug Design and Versatile Synthesis Process Development for TZD and Quinazoline Derivatives

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ABSTRACT

Nature has provided us organic and inorganic compounds which are being used as therapeutic drugs since the beginning of human civilization. Organic compounds constitute a major part of these drugs. Owing to the unmet demand and quick relief from pain; we are utilizing synthetic compounds as drugs since nineteenth century. Synthesis of novel heterocyclic in laboratory has revolutionary changed the course of medical science. Hence, the development of novel heterocyclic compounds with desired efficacy and cost-efficient chemical processes is the major challenge and noteworthy task for 21st century. Therefore, I will discuss about my research in designing and synthesis of some novel heterocyclic compounds. An efficient and scalable approach for the synthesis of piperazine based glitazone derivatives has been explored. We have also developed one-pot sequential synthesis of quinazolin-8-ol derivatives employing heterogeneous catalyst for Suzuki-Miyaura coupling. Another major hurdle in drug development is declined in success approval of new medicines since decades despite the modern research tools. Biopharmaceutical issues like PK and bioavailability is one of the major reasons for this. It has been found that more than 30% of molecules designed shows activities during Invitro/preliminary studies but the ratio decreases sharply due to poor biological profiles. Therefore, researchers are focusing on controlled drug delivery of target molecules. Conventional drug administration often requires high dosages or repeated administration to stimulate a therapeutic effect; this can lower overall efficacy and patient compliance which result in severe side effects and even toxicity. At the end of my talk, I will explain how controlled drug release can address such issue.

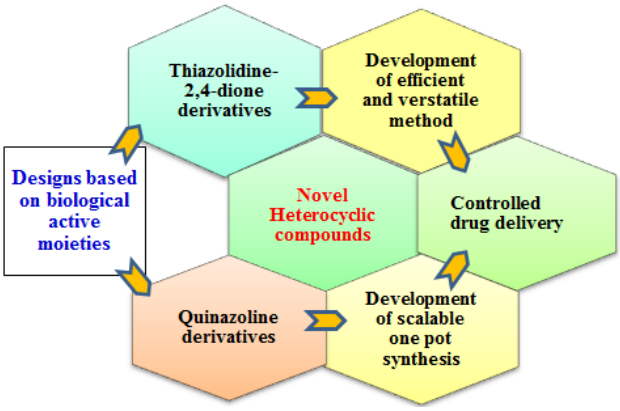

Fig. 1. Graphical summary

ORAL PRESENTATION

Characterization of Metal Organic Frameworks: The Building of Robust Structures

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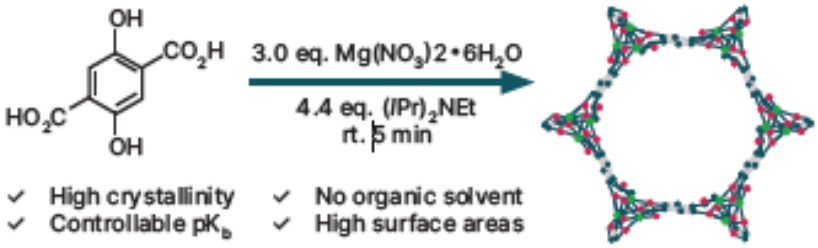
ABSTRACT

Metal Organic Frameworks (MOF's) are crystalline hybrid materials created from both organic and inorganic molecules by molecular self-assembly. Due to their porous structure, MOF's have an extraordinarily large internal surface area that gives rise to many interesting properties, for example, improved selectivity, higher loading capabilities and robustness in catalytic reactions.



MOF cage-like structures have opened the door to numerous applications in many fields that exploit the unique architecture of the crystalline structures in these materials.

Reproducibility and stability of MOF structures are critical to the properties that are required for these materials to maintain their robust performance. In this paper, we will show a variety of example MOF applications and review some key characterization methods such as X-ray diffraction, static and dynamic light scattering, zeta potential and image analysis.

Keywords: Metal Organic Frameworks (MOF's), Cage-like structures. Reproducibility.

OP2

Microwave Assisted Synthesis of Pseudo Ladder Mono Hydroxy Pendant PolyBenzobisthiazole Thermoplastic Polymer

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ABSTRACT

Green chemistry requires the use of less dangerous raw materials and modifications to conventional chemical production. Green chemistry strives to increase the effectiveness of synthetic processes while utilizing less hazardous solvents, fewer stages, and as little waste as is practically feasible. We execute MW-assisted synthesis of a novel, high performance PBZT polymer that contains pendent hydroxyl moieties with this in mind and in an effort to shorten the process time. The claim that MW-assisted synthesis is a quick synthesis method is true. By minimizing the generation of undesirable byproducts during the reactions, the MW-assisted synthesis has significantly decreased the reaction time and increased product yields. We performed Anisotropic polymerization of 5-hydroxy isophthalic acid and isophthalic acid with 2,5-diamino 1,4-benzene dithiol dihydrochloride (DABDT.2 HCl) affords the polymer poly {[benzo (1,2-d: 4,5-d') bisthiazole-2, 6 diyl]-1,3 phenylene} and poly {[benzo (1,2-d: 4,5-d') bisthiazole-2, 6 diyl]-1,3(5-hydroxy phenylene)}. Both of the polymers were soluble in methanesulphonic acid and chlorosulphonic acid. The polybenzobisthiazoles do not exhibit any glass transition temperature (Tg) by DSC analysis. Thermo gravimetric analysis indicated that the polybenzobisthiazoles were stable up to 400^0 C in nitrogen atmosphere. Polymer structures were verified by elemental analysis and spectroscopic comparison of polymers with appropriate model compounds. Inherent viscosity of the polymers was up to 4.2 dL/g (methanesulphonic acid, 30^0C).

Keywords: MW-assisted synthesis, Pseudo ladder; Polybenzobisthiazole; Anisotropic polymerization. polymers; copolymers)

OP3

Co(II) and Ni(II) Complexes as Electrocatalysts for Proton Reduction

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ABSTRACT

Solar energy harnessing is a promising way to meet the increasing global energy needs. An important approach in this context is artificial photosynthesis (AP) wherein water is split into hydrogen and oxygen using electrocatalysts incorporating different chromophores.[8-9] For the reductive side of AP (H_2 generation), a highly active catalyst, stable in the presence of water and designed using earth abundant materials is preferable. Identifying a robust, active, and efficient electrocatalyst is hence, a crucial first step in this direction. Though Pt is active for proton reduction, the widespread application of Pt is limited due to its rare nature. Keeping this in mind, efforts have focused on using abundant elements such as Fe, Co, Ni, Mo and different combinations of ligands for designing the proton reduction catalysts. For the ligand platforms in developing the catalysts with inexpensive components, Schiff base ligands have received special attention in the past few years.

Based on the above-mentioned facts, tetradentate Schiff base ligands N, N'- Bis (salicyldiene) ethylenediamine (**L^1**),2,2'-((1E-1'E)-(ethane1,2diylbis(azanylyidene))bis(ethane-1-yl-1-ylidene))diphenol(**L^2**) and 3-(2-(E)-(hydroxynaphthyl)methyl)imido)propylamine) (**L^3**) were reacted with $MCl_2.6H_2O$ (M = Co, Ni). The synthesized Schiff base complexes [Co^{II}(**L^1/L^2/L^3**)] **1-3** and [Ni^{II}(**L^1/L^2/L^3**)] **4-6** were characterized by FTIR, NMR and UV-Vis spectroscopic techniques, mass spectrometry, elemental, and thermal analysis. The reported complexes **1**, **2**, **4-6** and the new complex **3** were investigated for electrocatalytic proton reduction to dihydrogen in the presence of weak acid (acetic acid) in homogenous media (CH_3CN).

OP4

Quinazolin-4-(3H)-one Derivatives as an Anticancer Agent

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ABSTRACT

Nitrogen containing heterocyclic compounds are having very important role in the field of medicinal chemistry. Quinazolin-4-(3H)-none derivatives are one of them which are shown amazing broad spectrum as an anticancer agents. There are many Quinazolin-4-(3H)-none analogues were synthesized and characterized by different analytical techniques such as LCMS (Liquid chromatography mass spectra), IR spectroscopy, NMR (nuclear magnetic radiation), Gas chromatography, Melting point, SOR (Specific optical rotation), etc. The Quinazolin-4-(3H)-none derivatives were evaluated for their cytotoxic activity on different type of human tumor cell lines such as HeLa (Cervical cancer), MCF-7 (Breast cancer), HL-60 (Human promyelocytic leukemia) and HepG2 (Hepatocellular carcinoma), A2780 (Ovarian Cancer), NCI-H460 (non-small cell lung cancer) and HCT-15 (colorectal adenocarcinoma) at different concentrations. They exhibit in vitro cytotoxic activity in the low micromolar range and showed good molecular docking score. Structural activity relationship of these compounds revealed that the Quinazolin-4-(3H)-none has gained momentum recently. The motive of this study is to provide an overview of anti-cancer activity of various Quinazolin-4-(3H)-none derivatives, so that it could be a new class of anticancer agent.

OP5

Exploring the Potential of Polyurethane Adhesive Towards Laminating Dual Metallised Polyester with Different Substrates for Reflecting Radiative Heat

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ABSTRACT

The present work aims at developing the outermost layer of fire proximity clothing using a non-halogenated fire-retardant polyurethane-based adhesive. Polyurethane was prepared by the chain extension of an MDI based prepolymer with butanediol, with the former being a reaction product of MDI with polycaprolactone diol in the presence of trimethylol propane. Subsequently, a non-halogenated fire retardant was used to introduce fire retardancy to the polyurethane, and the same was used as an adhesive for laminating a dual metallised polyester film (optical density 4.8) with a glass fabric (sateen weave, 390 gsm). The requisite level of adhesion in the developed laminated was demonstrated by placing it in hot water (60 °C) for a period of 15 min followed by flexing operations for a predetermined number of flex cycles. The developed laminate could withstand 1000 cycles of flexing, with no evidence of cracking or delamination. The flexible nature of the laminate was quantified in terms of its bending rigidity in both warp and weft directions. It is to be noted that the developed reflective laminate is destined for use as an outer layer in proximity clothing, where a distinct possibility of the removal of the deposited aluminium exists during service operations. In view of the same, the radiative performance was determined after 300 cycles of abrasion with a cotton abradant. The radiative heat transfer index (RTI_{24}) of the laminate was found to be ~28s. Further, a multi-layer component assembly was prepared by combining the developed reflective laminate with a moisture barrier, thermal barrier and an inner lining and the same was subjected to a convective heat flux. The increase in temperature as a function of exposure period was plotted and the time associated with the intersection of Stoll curve was used to quantify the extent of protection offered to second degree burns. The developed configuration offered a protection to 2^{nd} degree burn for a period of 35 sec, which clearly highlights the potential of the laminate as a reflective layer in fire proximity clothing.

OP6

Pyridine Based Anti-microbial Derived from Para-benzoquinone with Chloro Terminated from Benzimidazole

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ABSTRACT

In the recent few years, the study of antimicrobial drugs and their pharmacology has been a major interest field for the researchers. While their medical proportion has dramatically increased, microbial infections also have grown to be a significant medical concern for human beings. Some novel pyridine-based derivative of tetrachloro-p-benzoquinone is synthesized by thermal heating method. The pharmacological activity of pyridine derivatives against many biological targets ranges from good to exceptional cures. With different substituents on the pyridine nucleus, different malignant cells, viral infections, and microbial diseases are all potential biological targets. Pyridine derivatives interact with enzymes, proteins, and DNA to target numerous biological disorders. Further the synthesized moieties have been reacted with chloro derivative of benzimidazole. The structural confirmation will be supported by 1H and 13C nuclear magnetic resonance (NMR) spectroscopy, Fourier transform-infrared spectroscopy, and liquid chromatography-mass spectrometry. The synthesized derivatives have demonstrated remarkable biological activity against 5JLC (Structure of CYP51 from the pathogen Candida glabrata) by in silico molecular docking technique. In comparison to the renowned recognized drugs, the compounds have moderate to good biological activity.

***Keywords**:* Pyridine, Tetrachloro-p-benzoquinone, Molecular Docking, Anti-Microbial, Biologically Active.

OP7

Hybrid Photocatalyst for Hydrogen Production

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ABSTRACT

Solar power induced photocatalytic hydrogen production has an enormous potential to solve the energy crisis being faced by our generation. We have developed novel hybrid photocatalyst metal-oxide cluster-anions (polyoxometalates, or POMs) as covalently coordinated inorganic ligands on the anatase nanocrystals surfaces which is in continuation of our earlier work.[1] Sodium salts of the water-soluble polyanionic structures are obtained by reacting amorphous TiO_2(s) with the 1-nm size mono-defect Keggin ion, $Na_7[\alpha\text{-}PW_{11}O_{39}]$ at 140 °C. Metallic Ni NPs are decorated at the surface of the TiO_2-POM hybrids surfaces in order to prevent charge recombination which in turn will increase the hydrogen production efficiency during photocatalysis using methanol and water mixture. The hybrid materials were characterized using FTIR, XRD, SEM and Dry TEM techniques. All these techniques confirm the formation of novel TiO_2-POM-Ni hybrid nanocomposite.

[1]Raula et al., Angew. Chem. Int. Ed., (Hot Paper), 2015, 52, 12416-12421.

OP8

Comparative Study of Light Emitting Diode Curable and Self-Curable Dental Resin

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ABSTRACT

The main objective of this work was to analyze and match the various essential properties of two different kind of dental composite, one is self-cured dental resin and the other is cured with the help of light-emitting diode lamp (LED).

We selected two dental composites, one is a copolymer of acrylic and itaconic acid and the other is a bisphenol-A -glycidyl methacrylate (Bis-GMA) grafted copolymer. The copolymer is self-cured in more than 2 minutes while grafting of Bis-GMA on copolymer is LED curable that takes 20 seconds for curing in the presence of photoinitiator (Camphorquinone). FTIR was used to determine the functional group in resin. Dental resin mix with 20 micron size fluoro- aluminosilicate powder in 2:1 ratio specimen were prepared (6mm+ 0.1mm high and 4mm+ 0.1mm diameter) for compressive strength. Scanning Electron Microscopic (SEM) analysis of cured resin was carried out for surface morphology.

FTIR confirmed the presence of unsaturation in LED-cured dental resin which makes it light sensitive, while self-cured dental resin is completely saturated. Compressive and flexural strength shows that LED cured dental resin has higher strength than self-cured dental resin. SEM images confirmed a smoother surface of LED cured resin than self-cured.

LED cured dental resin has an exclusive combination of prolonged working time and very short setting time achieved by exposure to LED light. Polymerization by LED light exposure not only provide a shorter setting time but also enhanced mechanical and physical properties as compared to self-cured resin.

Keywords: Compressive strength, light-cured, self-cured

OP9

Evaluation of Dye Degradation Using Phosphorous Doped g-C_3N_4

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ABSTRACT

Graphitic carbon nitride (g-C_3N_4) is an exciting conjugated polymeric material. It is a new area of research and has drawn interest from many different fields as a metal-free and visible-light-responsive photocatalyst in the fields of solar energy generation and ecological restoration. This can be attributed to its "earth-abundant" character, great physicochemical strength and durability, and attractive electronic band arrangement. Authors have synthesized P-doped g-C_3N_4 using the thermolysis method. Morphological studies such as FESEM, EDX, and XRD confirm the synthesis of P-doped g-C_3N_4. The photoelectrochemical and photocatalytic studies confirm that P-doped g-C_3N_4 shows better photocatalytic activity than pure g-C_3N_4. This is due to the most favourable morphology, least charge-transfer resistance, most facile kinetics, most negative flat band potential, and least recombination of electrons and holes, which can lead to maximum photoactivity towards dye degradation by P-doped g-C_3N_4.

OP10

Synthesis and Physicochemical Assessment of Anionic Polymeric Surfactant from Palm Oil for Improved Oil Recovery

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ABSTRACT

The synthesis of polymer grafted anionic surfactant (PMES) using non-edible vegetable oil (palm) as the source material with the intention of using it in enhanced oil recovery (EOR) has been the primary emphasis of this research. The polymeric surfactant was created through a process known as free radical polymerization, which involved the reaction of acrylamide monomer and methyl ester sulfonate (MES), which was synthesized from palm oil. The mobility ratio can be regulated by a polymeric surfactant with characteristics of both a surfactant and a polymer, and the interfacial tension (IFT) can be decreased, both of which are beneficial for EOR. The techniques of FTIR were utilized in order to investigate the characterization of polymeric surfactant. The effectiveness of PMES in the cEOR (chemically enhanced oil recovery) process was investigated by measuring the physiochemical characteristics of its aqueous solution, namely a reduction in the amount of initial fractional temperature (IFT). These investigations were carried out with the purpose of evaluating PMES in terms of its potential application in enhanced oil recovery.

OP11

3D-QSAR Based, Pharmacophore Modelling, Virtual Screening, and Molecular Docking Studies for L-type Calcium (LTCC) in Iron Overload in β-thalassemia

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ABSTRACT

Excessive body iron, also known as iron overload, occurred in thalassemia patients who are dependent on blood transfusion treatment. Iron overload causes, iron accumulation in a variety of tissues, particularly the liver, brain, heart, and endocrine tissues. Arrhythmias, dilated cardiomyopathy, and diastolic failure are all caused by elevated cardiac iron. Iron removal with the iron-chelating agent is the primary strategy for the treatment of iron overload. Deferasirox has been used in humans for nearly half a century; however, it is less favoured by patients due to intravenous administration and adverse effects. L-type calcium channel (LTCC) blockers have been shown to reduce iron excess in cardiomyocytes, liver cells, and nerve cells. The uptake of non-transferrin-bound iron (NTBI) in rat ventricular myocytes has been demonstrated to be mediated by the L-type calcium channel (LTCC). In iron-overloaded animal models, the LTCC blocker nifedipine can suppress iron overload-mediated hepatocyte apoptosis and increase urine iron excretion. LTCC inhibitors additionally have a part in regulating renal iron transport. This in-silico work utilised bioactivity value (IC_{50} value) of known inhibitors for 3D QSAR pharmacophore model preparation. The selected models were used to screen library and validated using a test-set of compounds. Best Hit molecules were further investigated using virtual screening and molecular docking analysis. The top ranked candidates were tested for toxicity, and their inhibitory activity and iron chelation efficacy were predicted. At last top most chemical compounds were obtained with optimised docking score, low estimate value and acceptable toxicity and ADMET profiling.

OP12

Synthesis and Structural Characterization of Schiff Base Based Transition Metal Complexes

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ABSTRACT

In this study, two complexes [Co(C7H9N3S2)2Cl2]Cl2, and [Ni(C7H9N3S2)2Cl2]Cl2 were synthesized from 2-Acetyl thiophene thiosemicarbazone (C7H9N3S2) respectively and characterized using various characterization techniques. 2-Acetyl thiophene thiosemicarbazone (L) was prepared using 2-Acetyl thiophene and thiosemicarbazide. [Co(C7H9N3S2)2Cl2]Cl2 and [Ni(C7H9N3S2)2Cl2]Cl2 was synthesized using the 2 moles of 2-Acetyl thiophene thiosemicarbazone and one mole of either CoCl2 or NiCl2 salt. The study of magnetic moment (4.92 B.M. for [Co(C7H9N3S2)2Cl2]Cl2) and (2.93 B.M. for [Ni(C7H9N3S2)2Cl2]Cl2) showed that both complexes are paramagnetic in nature. The value of electrical conductance (184 Ohm^{-1} cm^2 $mole^{-1}$ for [Co(C7H9N3S2)2Cl2]Cl2 and (173 Ohm^{-1} cm^2 $mole^{-1}$ for [Ni(C7H9N3S2)2Cl2]Cl2) suggested that that the two equivalent of the ligand is attached to the metal ions. The electronic spectrum data (8000-8650, 20800-21580, and 16200-17500 cm^{-1}) suggested that the [Co(C7H9N3S2)2Cl2]Cl2 spin-free octahedral complex. The electronic spectrum data (9500-10415, 14200-14940, and 23500-24000 cm^{-1}) suggested that the [Ni(C7H9N3S2)2Cl2]Cl2 is in an octahedral geometry. An IR study showed that ligand is coordinated to the metal via nitrogen atoms of C=N-, and sulfur atoms of C=S-. The vibration bands of νM-Cl at 325-350 cm^{-1} confirm that Cl^- ion is also coordinated with the metal ion. This study confirms the synthesis, and structure of new metal complexes [Co(C7H9N3S2)2Cl2]Cl2 and [Ni(C7H9N3S2)2Cl2]Cl2.

OP13

Design, Synthesis and Pharmacology of Some Oxadiazole Derivatives and Their S-Glucosides Bearing Thaizole Scaffold

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ABSTRACT

In a search of new anti-cancer and anti-malarial agent a series of 5((4(substituted-phenylthiazol-2-yl) thio) methyl)1,3,4 oxadiazole2-thiol and their S-glycoside incorporating thiazole. S-Glycosides, which are serve as enzyme inhibitors, are crucial tools for determining specific protein-carbohydrate interactions and can greatly help structural and functional studies of carbohydrate-active enzymes. All compounds are assayed for their bonding in the active site *of human T-cell leukemia virus protease*, a novel target for anti-cancer (PDB ID-2B7F) study. The oxadiazole derivatives showed negative binding energies promising potent inhibitory activity. The compounds were synthesized and characterized by spectral analysis (^{1}H-NMR, ^{13}C-NMR, Mass, and FT-IR) and elemental analysis. In the present communication an attempt is made to cover the medicinally active compounds along with recent synthesis, which were reported to possess antimicrobial and antifungal activity.

OP14

Comparative Adsorption Study of Heavy Metals on Ferrites Synthesised by sol-gel and Co-precipitation Methods

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ABSTRACT

In the present work, cobalt and zinc ferrites synthesised by sol-gel and co-precipitation method using precursors as nitrates, chlorides and urea. Characterization of these ferrites done using X-Ray Diffraction (XRD), BET and Fourier Transform Infrared Spectroscopy (FTIR). Adsorption of nickel and copper were studied on both cobalt and zinc ferrites with the help of UV-Visible absorption spectrophotometer. The adsorption was studied with varying pH of metal solution and contact time of ferrites with metals. It was studied against the adsorption on activated charcoal. Finally, comparison of both ferrites on adsorption capacity of heavy metals was done.

Keywords: Ferrites, XRD, BET, FTIR, Adsorption

OP15

Facile Low Temperature Synthesis of Bismuth Molybdate Stabilized Ferricyanide and Ferrocyanide Nanocomposites

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ABSTRACT

Recently, the development of environment friendly and green solutions to remediate water resource pollution has received global attention. Bismuth molybdates are considered among the most intriguing materials, due to their unique characteristics and emerging demands, such as ion conductors, photoconductors, sensors, photocatalysts etc. Owing to their outstanding employment, we aimed to fabricate the visible light active bismuth molybdate stabilized ferricyanide and ferrocyanide nanocomposites. The structural and spectrophotometric results indicated that the prepared composites have an orthorhombic crystal structure and the band gap energy of 2.95 and 2.78 eV respectively. The nanocomposites were synthesised through one step hydrolysis method. The nanocomposites were tested to lab-scale photodegradation of Methyl Orange (MO) under visible light irradiation. The photocatalytic results demonstrated that the coordination complex of BMO/Ferricyanide and BMO/Ferrocyanide in the present study showed much enhanced photocatalytic performance and degraded 62% and 76% of MO, respectively.

OP16

Design, Synthesis and Pharmacological Evaluation of Oxospiro Chromane Triazole Based Molecular Hybrids as Inhibitors of Acetylcholinesterase for the Treatment of Alzheimer's Disease

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ABSTRACT

With the aim of incorporating structure-based design to inhibit disease causing factors in the multifactorial Alzheimer's disease (AD), a series of new oxospiro chromane-triazole based molecular hybrids were designed and lead molecular hybrids were synthesized using spirocyclisation and click chemistry as the key steps in a convergent style. The molecular architecture of designed hybrids is expected to be potential inhibitors of acetylcholinesterase and promising beta-amyloid disaggregator in the AD therapeutics. Furthermore, the synthesized compounds were characterised using ^{1}HNMR, ^{13}CNMR and high-resolution mass spectrometry. In-silico study of hybrid molecules showed promising docking score as compared to mainstay FDA approved drugs. In addition, biochemical assay is under process which would be followed by molecular dynamic simulation to shed light on the mechanism of action of these inhibitors.

Keywords: Alzheimer's disease, Acetylcholinesterase, Anti-Neurodegenerative

OP17

Synergystic Effect of Solvent and Gamma Radiation on Ferrites as a Adsorbate for Methyl Orange Dye Removal

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ABSTRACT

Metal doped ferrites have major applications in environmental remediation. In this study, magnesium doped zinc ferrites $Mg_xZn_{(1-x)}Fe_2O_4$ were prepared by sol-gel auto-combustion method. These were characterized by X-ray Diffraction (XRD) and Fourier –Transform Infra-red Spectroscopy (FTIR) techniques respectively. The doped ferrites were synthesized in two different solvents viz, double distilled water and aloe vera gel. $Mg_{0.5}Zn_{0.5}Fe_2O_4$ was prepared using standard methods of synthesis. Both the synthesized doped ferrites were gamma irradiated with 50 kGy and 300 kGy doses and were again characterized using XRD and FTIR techniques to study the changes in structural properties of the ferrites. The effect of two different doses of gamma radiation on ferrites is compared using XRD and IR spectra. Structural changes were investigated in the doped ferrites post irradiation. Adsorption of methyl orange dye in water was studied using irradiated and unirradiated $Mg_{0.5}Zn_{0.5}Fe_2O_4$ ferrites under varying pH and time against a standard activated charcoal.

Keywords: magnesium doped zinc ferrite, XRD, FTIR, gamma irradiation, adsorption of methyl orange dye

OP18

Structure based Design and Synthesis of Bedaquiline Analogues as an Anti-Infectious Agents

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ABSTRACT

Millions of individuals are affected by infectious diseases like tuberculosis, which puts a heavy cost on society and presents a serious issue. Diarylquinolines have gained attention because of their application in the treatment of MDR-TB. Approval of Bedaquiline from diarylquinoline class was accelerated in 2012 but this drug associated with few limitations like high lipophilicity and cardiotoxicity. Therefore, with the aim to minimize associated limitations, here, we propose the design of new bedaquiline analogues utilising computational biology tools like Molecular Docking followed by chemical synthesis. The optimized analogues were docked into the binding pocket of ATPase to calculate the binding free energy and the protein-ligand interactions of the potent inhibitors were visualized. Preliminary computational studies are encouraging and the synthesis work is going on.

Keywords: Bedaquiline, ATPase inhibitors, Anti-Infectious agents, Molecular Docking.

OP19

Synthesis of 2-benzyl-1H-benzimidazole Derivatives and their Applications

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ABSTRACT

This work reports a novel synthesis and characterization of 2-benzylbenzimidazole derivatives under different conditions. Based on the recent report, 2-benzylbenzimidazole is chosen for our study as there is no such reported study available for N-substituted derivatives. We assume that N-substituted derivatives will provide novel results those can be tested biologically later as Benzimidazole derivatives exhibit pharmacological activities such as anti-tuberculosis, anti-malarial, antihistamine, antimicrobial, antiviral, antidiabetic, anticancer, anti-fungal, anti-inflammatory, analgesic, anti-HIV, etc. Core intermediate and few derivatives have been synthesized and the synthesis of more derivatives will be completed by Michael type reaction, alkylation or using other modified conditions. Few intermediates were synthesized using acrylates and 3-methylenepyrrolidine-2,5-dione derivatives.

***Keywords**:* Benzimidazole, Alkylation, Michael reaction.

POSTER PRESENTATION

Differential Salt Effects on Solubility and Aggregation Behaviour of Surfactant Molecules

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ABSTRACT

Inorganic salts have great impact on the solubility, stability, and even morphological parameters such as size and shape of macromolecules dissolved in aqueous medium. Detailed mechanistic information regarding these specific salt effects are yet to be fully understood and resolved. Surfactants, similar to large macromolecules like proteins, polymers and nanomaterials, show prominent salt effects in all of their applications. In this research work, aggregation phenomenon of a positively charged surfactant, CTAB, was systematically investigated in the presence of wide variety of dissolved salts using conductivity measurements. Different sodium salts were chosen for this purpose and their effect on critical micelle concentration of CTAB was recorded at a specified temperature. It was observed that highly charged kosmotropic ions such as sulphate have completely different interaction mechanism than that of less charge density chaotropic ions like iodide. Relative importance of the surfactant hydrophobic chain, identity of the charged head group and salt impact on the surface and bulk water structure in driving these observed salt effects was also carefully explored.

Keywords: Surfactant aggregation, critical micelle concentration, salt effects on water structure.

Diverse Methods for the Synthesis of Modified Chitosan Beads and Their Applications

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ABSTRACT

Chitosan is the second most abundant biopolymer on earth and is produced by deacetylation of chitin. Higher the degree of deacetylation, higher the adsorption capacity. Chitin is extracted from the exoskeleton of creatures such as lobster, prawns, crab etc. This review provides an overview of traditionally used and recently developed method for the preparation and modification of chitosan-based beads. Modification can be done by two ways physical and chemical process. Beads come under physical modification that enhances the porosity and surface area It also helps to expand chitosan polymer chains thereby increasing access to internal sorption capacity. Crosslinking, surface impregnation and grafting comes under the category of chemical modification. This process helps to bring new derivatives with improved properties without changing the basic structure. Further, the advances in the most recent years in their application are discussed. Chitosan beads are favourable adsorbents and could be employed as low-cost alternatives for the removal of dyes, heavy metals from the wastewater treatment because of the presence of many functional groups on it.

Keywords: Chitosan, modification, water treatment, pollutants.

Recent Advancement in 2-Dimensional Nanomaterials Based Flexible Strain Sensors and Future Challenges

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ABSTRACT

Strain sensors plays an important role in a wide range of applications such as structural health monitoring, and human movement detection. The conventional metal-based strain sensors suffer from difficult processing methods, flexibility problems, and low sensitivity. Gauge Factor (GF), the relative change in resistance divided by strain is a crucial parameter to characterize the strain sensors. Two-dimensional (2D) materials such as graphene, molybdenum disulphide, tungsten disulphide, and MXenes, have emerged as a platform of enormous possibilities in material science due to their distinctive electronic, mechanical, chemical, and optical properties. High surface to volume ratio, extraordinary mechanical, and electrical properties make them promising candidate for a new generation strain sensing device. In this paper, a comprehensive review of 2D materials-based strain sensor is reported, which mainly focuses on the recent development of 2D materials for strain sensing applications, synthesis, and properties. The future challenges of these prepared strain sensors are also highlighted.

Detailed work of this review will be presented during the symposium.

Keywords: Strain sensor; 2D nanomaterials; graphene; molybdenum disulphide; tungsten disulphide; MXenes

Floating Catalyst Chemical Vapour Deposition Derived CNT Aerogel for Oil Separation Application

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ABSTRACT

Oil spillage has been a common outcome of the rising developments of technologies and has an adverse effect to aquatic biodiversity and humankind. Various adsorbents have been developed to tackle the situation, however are often limited in their performance and usability conditions. The superior properties of carbon nanotubes (CNTs) including their mechanical stability, porous structure and large surface area have prompted their use as oil adsorbents. Indeed great results have been identified with the use of CNT coatings on spongy materials, their efficiency can be improved with elimination of hetero-material.

In this study, pristine CNT aerogel have been synthesized using floating catalyst chemical vapor deposition technique and have been used as an adsorbent for separating oil from water. For further improvements, additional pores have been introduced via chemical treatment and mechanical stability. The studies have been carried out on various oils including mustard oil, silicone oil, engine oil, castor oil, coal tar oil and chloroform and their adsorption capacities have been evaluated. The samples have also been tested for their regeneration performances and showed some positive results.

Synthesis and Fabrication of Metal Organic Framework Based Sensors for the Detection of Pesticides

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ABSTRACT

Pesticides are one of the major agrowaste that can disrupt crucial physiological processes of body, the effect of which is amplified due to bioaccumulation. Metal organic frameworks are highly ordered crystalline solids formed by coordination of metal ion and organic ligands, these fascinating materials are well known for their high porosity, catalytic activity, structural diversity, ease of fabrication and processibility enables them to interact with wide range of analytes, qualifying them to be suitable base material for pesticide sensing. Florescent MOF based analyte sensing have recently flooded the scientific literature, although due to lack of earlier design strategies not much have been discussed regarding electrochemical sensing capabilities of MOFs. In this review we aim to introduce recent work in MOF sensors for detection of pesticides with focus on synthesis strategies of MOFs and fabrication strategies.

Keywords: MOF's, Pesticides, Synthesis, Sensors.

Exploring the Thermoelectric Properties of MWCNTs Films Prepared by FCCVD Technique

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ABSTRACT

Flexible thermoelectric (TE) technology has enormous potential in the field of renewable energy. Conventional thermoelectrics has evolved through inorganic materials which poses toxicity, availability and low surface coverage issues. In this regard, flexible thermoelectric devices improve the heat-to-electricity efficiency and minimize the heat loss between TE devices. They have great potentials to provide a continuous power supply for wearable applications, and hence used in place of inorganic TE materials. Carbon nanotubes (CNTs), owing to their variable band gaps, and excellent electrical and mechanical properties, perform well as flexible p-type TE materials. However, their conversion to high performance n-type material is still a challenge in present text.

In this study, various combinations of amine dopants have been used to prepare doped CNT sheets with high negative Seebeck coefficients. Floating catalyst chemical vapor deposition (FCCVD) technique have been employed for synthesizing pristine CNT sheets. These sheets are then doped with combinations of PEI, DETA, and TETA to convert these naturally p-type substances into n-type materials. The presence of n-type dopant in these samples is confirmed by FTIR (Fourier transform Infrared spectroscopy) technique. To determine the thermoelectric property of these samples, the Seebeck coefficient is also calculated by an in-house prepared setup.

Half Heusler as a Promising Candidate for Mid-temperature Thermoelectric Applications

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ABSTRACT

Of the many existing forms of renewable energy, thermoelectric materials are advantageous for they convert wasted heat energy into electricity and eventually prevent global warming as well as meet the worldwide needs of energy. Thermoelectric materials have been in use for many years and their applications is reportedly found in space industry, automobiles, in aircrafts and many more. Despite many existing applications, thermoelectric materials have could not influence the day-to-day life. The wide applicability of thermoelectric devices is restricted by their low efficiency and cost, therefore researcher in the field of thermoelectric are continuously giving their efforts to develop high-efficiency and cost-effective thermoelectric materials. The most abundant waste heat with an effective recovery potential in our environment is in mid temperature regime ~ (500 - 900 K). Among the large categories of thermoelectric materials half-Heusler compounds could be more promising for thermoelectric applications owing to their imitable characteristics such as good electrical transport properties, excellent mechanical robustness, high chemical, and thermal stability as well as they are composed of cost-effective and less toxic materials. However, their high thermal conductivity is a matter of concern while using it as TE materials. Their thermoelectric performance may be improved by the synergistic tuning of electronic energy states and defect engineering. In this study, we have surveyed current status and future aspects of Half-Heusler alloys.

Development of Hybrid Photoactive Catalysts for Accelerating Organic Reactions

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ABSTRACT

A nanocomposite photocatalytic material mesoporous silica/g-C_3N_4, has been synthesised and the organic-inorganic hybrid composite thus formed shows substantial reduction ability of toxic organic pollutants (POPs) to industrially significant chemicals. POPs are predominant pollutants consisting of industrial chemicals (Polybrominated diphenyl ethers, polychlorinated biphenyls, polychlorinated biphenyls etc.), pesticides, and by-products of industries (furans and dioxins). They bio-accumulate in the food chain thereby creating a number of health risks and environmental impacts. The catalyst has been prepared through an incipient wet impregnation approach where mesoporous silica and melamine has been mechanically pulverized. This is followed by calcination of this mixture at 550°C for 4 h in air atmosphere. The developed catalyst has been characterized for its structural, thermal, textural characteristics. Further, the catalyst has been employed to perform photoreduction of POPs which has been monitored using UV-Vis spectroscopy. Control reactions have been additionally performed to investigate the influence of catalytic support, as well as the active catalyst.

Keywords: Silica, Photo-reduction, Carbon Nitride

Exploring Cellulose as a Low-Cost Precursor for Carbon Nanofibers: A Study on Synthesis Optimization and Characterization

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ABSTRACT

Carbon fibers are highly sophisticated materials with diverse applications in structural and energy fields. PAN, Rayon, and Pitch are the primary precursors for carbon fibers, among which PAN is the most widely used due to its high carbon content, excellent tensile strength, and thermal stability. However, the high cost of precursor PAN and the harmful emissions during carbon nanofiber manufacturing have limited their use. Therefore, researchers are exploring low-cost alternative precursors, such as lignin and cellulose, which have high carbon content and are readily available in nature. In this study, we investigate the use of cellulose as a precursor for carbon nanofiber synthesis using the electrospinning technique. We optimized the process parameters to obtain the desired fiber morphology and diameter. Additionally, we employed vacuum-assisted deacetylation to reduce the conversion time of cellulose acetate to cellulose nanofiber sheets. The resulting nanofibers were characterized using analytical techniques, including Optical microscopy, FT-IR, XRD, and RAMAN measurements, to determine their structural and morphological properties. Our findings suggest that cellulose is a promising low-cost precursor for carbon nanofiber synthesis, and the electrospinning technique offers a promising approach to producing high-quality carbon nanofibers with desirable characteristics for various applications.

Synthesis of Metal Telluride Nanomaterials and Their Application in the Catalysis

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ABSTRACT

Nanotechnology is an emerging field in the material science community. Metal telluride nanomaterials have attracted noteworthy attention in the last few decades. It is one of the most explored groups of nanomaterials because of its remarkable surface chemistry. Another major reason for the popularity of nanomaterials is their unmatched properties like electronic, chemical, and optical properties. Due to these properties, they have a high capability to be used in the field of catalysis. solar energy conversion, magnetic, and many other areas. In this report, various shape and size-controlled nanomaterials synthesis methods have been discussed. Different shapes and sizes of Metal Telluride nanomaterials affect their activities in the catalyst. Applications of nanomaterials vary with their shape and size, some of them are antioxidant and catalytic applications. Here, our main aim is to synthesize nanomaterials of various shapes and sizes using capping agents by finding the simplest method available. Capping agents play an essential role in the controlled shape and size synthesis of metal telluride nanomaterials.

PP11

Synthesis of 1,4 Dihydropyridine Scaffolds and Evaluating them for Various Biological Activities

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ABSTRACT

1,4 Dihyridropyridine (1,4 DHP) has emerged as an exemplary pharmacophore nucleus over the last two decades and has consequently been incorparated in some viable commercially available drugs; with its bio-compatible nature followed by plethora of theraupatic and biological activities as antihypertensive, antileishmanial, antifungal, anti-diabatic, anticonvulsant, calcium channel antagonist, anticancer, anticoagulant, and antioxidant have grabbed the eyeballs of researchers.The classical method adopted for the synthesis of 1,4 DHP scaffolds is by Hantzch Mechanism involving condensation of an aldehyde, ethyl acetoacetate and ammonium acetate as a source of nitrogen leading to aromatization into a 1,4 DHP ring.The present work throws light on synthesis of novel scaffolds of 1,4 Dihydropyridine by adoption of such mechanism in a one pot , multicomponent ,solvent-free environment using $Ba(NO)_3$ as a catalyst. The product obtained was characterisated by ^{1}H-NMR and ^{13}C-NMR spectroscopic techniques followed by evaluation and interpretation of its biological activities.

Effect of Inter-conversion Reaction in Phase- Separation Kinetics of Isomeric Mixtures

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ABSTRACT

Inter-conversion can take place in isomeric mixtures, and it affects the phase separation kinetics and this affect is studied in this work. The work is completely computational. A model of such a system is constructed using a prototype of the Ising model, considered to be the fruit-fly model of "statistical mechanics". Such a model is investigated using Monte Carlo simulation in the semi-grand canonical ensemble. The kinetics of the phenomenon is understood by borrowing tools from the known techniques and results of non-equilibrium dynamics of phase transitions. Our focus in this work is on the growth law in case of isomers and how does it deviate from the growth law of pure phase separation kinetics.

Synthesis of Coumarins by Pechmann Condensation using Nano Ferrites

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ABSTRACT

Coumarin, a benzopyrone derivative, is naturally found in tonka beans and cinnamon. They are plant metabolites that protect plants from infections and help in plant growth, respiration, and photosynthesis. They are also reported to have important pharmacological properties such as antioxidants, anticancer agents, antiviral agents, antiviral agents, anti-HIV agents. It acts as a fluorescent dye and a plant metabolite. It has a pleasant smell like vanilla but is bitter in taste. Many methods have been developed to chemically synthesize coumarin which includes Perkin reaction, the Knoevenagel reaction, and the Pechmann reaction. The use of simple reactants like phenol and any beta keto-ester makes Pechmann condensation the most common method for the synthesis of coumarin in presence of any Lewis acid catalyst. In this paper, different coumarin derivatives have been synthesized by using the Pechmann reaction between different phenolic derivatives and ethyl acetoacetate. The reaction was catalyzed by nano ferrites of copper, nickel, manganese, and cobalt. The reaction was also carried out using conventional sulfuric acid as a catalyst. The structure of coumarin derivatives was confirmed by spectral analysis. Also, they imparted fluorescence in the UV chamber (at long wavelength ~365 nm) on TLC silica plates that suggest their possible applications as florescent tags in chemical reactions.

Keywords: Coumarin, Pechmann condensation, fluorescence, benzopyrone, nano ferrites

PP14

Multistep Synthesis, Isolation and Characterization of Impurities of Cardiovascular Drug Rosuvastatin

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ABSTRACT

In this project cardiovascular drug rosuvastatin (API) impurities are synthesized and isolated by Coloumn chromatography and novel stability-indicating reversed-phase high performance liquid Chromatography method. For the synthesis of rosuvastatin lactone impurity rosuvastatin free acid is refluxed overnight and purified using method Flash coloumn chromatography with tray size (18 X 150 mm) at 30 degree Celsius. Impurity rosuvastatin lactone (N-[4-(4-Fluorophenyl)- 6-(1-Methylethyl)-5-[(1E)-2-[(2S,4R)-tetrahydro-4-hydroxy-6-oxo-2H-pyran-2-yl]ethenyl]-2- Pyrimidinyl]-N-methyl-methanesulfonamide) is showing 98.16 percent area and the run time is 45.439 minute in HPLC. At 248 nm, all impurities are observed. Gradient elution mode is used to Separate impurities naming Anti-isomer, 5-ketoacid, lactone are all well-separate and its characterization with analytical techniques as NMR, Mass and IR is done.

PP15

Functionalized CNT Based Gas sensor with Low Detection Limit at Room Temperature

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ABSTRACT

Carbon nanotubes (CNTs) have a large surface area, making them a very sensitive detection element for a wide range of analytes present in ppb and ppm levels. Single-walled carbon nanotubes (SWCNTs) based gas sensing material was fabricated via modification of SWCNTs with polyethylene glycol (PEG) and poly-amino benzoic sulphate (PABS). The PEG and PABS modified SWCNTs increases its responsiveness. These functionalized SWCNTs based sensors were found to exhibit excellent sensitivity with high response, and low detection limit for gases such as nitrogen dioxide, ammonia. These functionalized SWCNTs are the promising materials for selective gas sensor at room temperature.

Synthesis of Benzodiazepinone and Benzimidazole Based Hybrid Molecules of Medicinal Interest

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ABSTRACT

The work represents the synthesis of Benzodiazepinone and Benzimidazole based Library of molecules as Antidepressants and Antiviral drugs with their physical as well as analysis results. Using modern synthesis designing library of scaffolds of Benzodiazepinone derivatives along with derivatives of benzimidazole acids (substituted) that are of medicinal interest. Use of costlier raw material followed by synthesis and purifying through washings and analysing through spectroscopic techniques. The work includes different sets of functional group transformation reaction for Benzodiazepinone synthesis simultaneously taking different sets of substituted benzaldehydes for synthesising Benzimidazole acid derivatives. The reactions are quite temperature sensitive and maintaining the optimum conditions leading to formation of fine product with healthier yield followed by washings with best solvents. Thin Layer Chromatography is the side running step revealing the reaction progress along with deciding the purity of the product. Little discussion related to Insilico-toxicology its introduction and its application. Through Literatures and Graphics glimpse of toxicology studies could be done. Through these techniques easy prediction on impact of drug on individual could be done.

De-nitrative Arylation of Nitrostyrenes with Aryldiazonium salts

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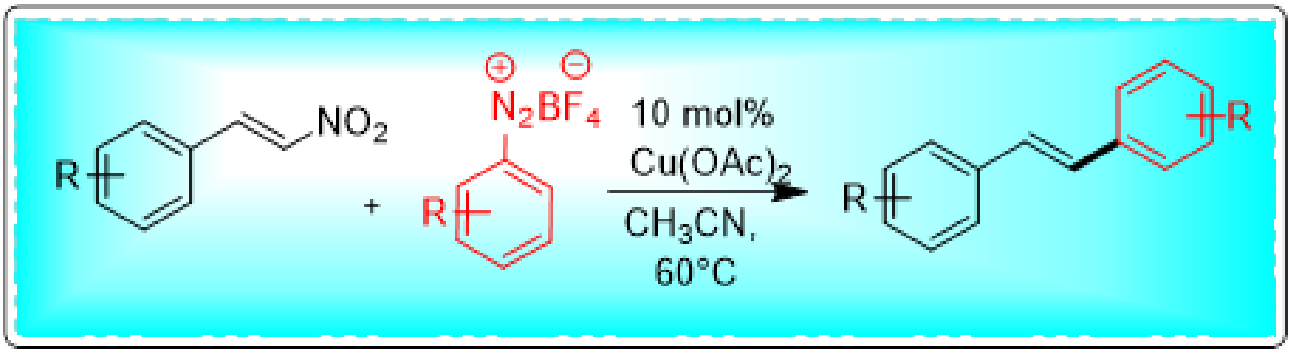
ABSTRACT

β-Nitrostyrenes constitute an important class of synthetic intermediates and hence, can also be explored as one of the coupling partners with diazonium salts using 10 mol% of Copper Acetate [$Cu(OAc)_2$].The versatility of the methodology under the established set of reaction conditions, the cross-coupling reaction of β-nitrostyrenes with diversely substituted diazonium salts to afford a variety of trans-stilbenes. The practical approach by varying the substituted β-nitrostyrenes with substituted diazonium salts which shows good functional group tolerance and were obtained in good yields. Following the protocol, we are pleased to mention that (E)-3,4,5,4′-Tetramethoxystilbene (DMU 212) was also synthesized which is a derivative of resveratrol with anti-angiogenic and anti-tumor properties. Still further mechanistic studies and applications of the synthesized compounds are under investigation.



Keywords: β-Nitrostyrenes, copper acetate [$Cu(OAc)_2$], diazonium salts, trans-stilbenes

PP18

MXenes: New Prospects in Catalysis

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ABSTRACT

Since last few decades, 2-dimensional (2D) transitional metal carbides (TMC), which are also known as MXenes have gained increasing attention in catalysis due to their tuneable morphologies, stability under certain conditions, many exciting properties such as excellent electrical and mechanical properties, hydrophilic behaviour due to functionalized surface, highly stable colloidal solution due to negative zeta potential, and adaptable electronic structures. MXenes are promising catalysts, and supports for electrocatalysis, heterogeneous catalysis, photocatalysis and biocatalysts. Here, we systematically discuss the various synthesis routes of the MXenes, briefly summarizes the most significant catalysis processes, specifically an alternative material for catalytic reactions, and different catalytic applications with a precise mechanism. Finally, we also discuss the exciting challenges faced and future aspects of MXenes as an all-round material in catalytic application. This material can provide the guidelines of efficient MXenes-based electrocatalysts for the future development of hydrogen production through water-splitting processes.

Detailed work of this review will be presented during the symposium.

Keywords: MXenes; catalysis; electrocatalysis; photoelectrocatalysis

Hydrocracking of Heavy Crude Oil using Ni-Mo Nanocatalyst in Slurry Phase Reactor

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ABSTRACT

Ever-rising demand of global energy as well as continuous reduction in the availability of light crudes, strongly desires attention of research community to make efforts in the direction of efficient utilization of extensively available heavy crude reserves. It is worth mentioning that heavy crude oil exhibits potential to meet the demands for high-value transportation fuels and industrially significant chemicals. Hydrocracking which is defined as a refining process of heavy crude oil as well as heavy fractions into lighter quality products and can be accomplished in slurry-phase type reactor. In the present work, variety of nanocatalysts based on Ni-Mo with different Ni & Mo molar ratios have been developed, via co-precipitation method and have been evaluated for its catalytic efficiency for hydrocracking in slurry phase reactor. Further, hydrocracking of heavy crude oil has been performed at 420°C, under 7.0 MPa of initial H_2 pressure in 4 hr. Followed by this, the reaction products were analyzed by utilizing techniques such as analysis of saturates, aromatics, resins, and asphaltenes (SARA) fractions, simulated distillation (SIMDIS), API gravity and sulphur contents, to investigate the influence of reducing nanocatalysts in hydrocracking.

Keywords: Catalyst, hydrocracking, sulphur content,

Recent Advancement in Nanotechnology Enabled Smart Sensors for Environmental Contaminants Detection

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ABSTRACT

Environmental pollution is a global issue that has a negative impact on socioeconomic development and human health. The presence of environmental contaminants such as pesticides, antibiotics, heavy metal ions, waterborne and foodborne diseases, and other hazardous substances poses serious public health risks. The nanotechnology enabled sensors has shown potential for rapid, specific, and highly sensitive detection of these contaminants. Nanomaterials incorporated nanosensors for environmental monitoring has several advantages over conventional detection methods, including improved sensitivity, selectivity, reliability, accuracy, and rapid detection capabilities. This review summarizes the recent development in nanotechnology based nanosensors which can monitor the environmental contaminants such as pesticides, antibiotics, heavy metal ions, waterborne and foodborne pathogens, and other toxic chemicals. The potential of nanosensors for improving public health and environmental sustainability are also discussed. The need for continued development and implementation of these technologies in environmental monitoring is also highlighted.

Keywords: nanomaterials; nanosensors; food monitoring; heavy metal ions; detection; pesticides; pathogens

PP21

Impurity Profiling of Antihyperglycemic Drug- Sitagliptin

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ABSTRACT

Sitagliptin is a type of antihyperglycemic drug that is commonly used for the treatment of type 2 diabetes. It is used to regulate uncontrolled sugar levels in the blood. It is a dipeptidyl peptidase-4 (DPP-4) inhibitor that represents a new therapeutic approach to reducing glucagon levels.

We present a simple, convenient, and efficient method for the synthesis of six impurities viz. Phenyl ethyl amine Impurity, Triazole impurity, acid impurity, alkene impurity, Cyclohexyl Impurity, Enantiomer Impurity in Sitagliptin by utilizing readily available starting materials. These impurities can be detected by utilizing simple techniques such as high-performance liquid chromatography (HPLC) and liquid chromatography-mass spectrometry (LC–MS), FTIR, and NMR (^{1}H and ^{13}C). All these synthesized impurities show their presence in the sitagliptin sample which can be confirmed by co-injection and matching the retention time with spiked impurities.

Impurities are used in pure form for validation of method specificity, Limit of Detection, Limit of quantification, robustness, and relative response Factor.

The degradation of Sitagliptin was also studied under acidic, basic, and oxidative conditions. Excipients used in the study i.e., fumaric acid, lactose showed interaction with Sitagliptin.

Keywords: Sitagliptin, Anti-diabetic, Impurities, LC-MS, FTIR, NMR, Degradation Product

Carrier Activation in Mg Doped GaN

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ABSTRACT

In this modern world, gallium nitride alloys are receiving immense applications due their wide band gap i.e. 3.4eV and high operating temperatures, high breakdown electric field. Gallium Nitride (GaN) and group III nitrides are auspicious materials in manufacturing of green, blue, violet LEDs and laser diodes (LDs). To forge such LEDs and LDs its necessary to achieve high carrier concentration in P type doped GaN. Magnesium (Mg) is the most suitable dopant due to low ionization energy and a shallow acceptor. In GaN power devices p-n junction is the important component. It has been reported that for n-type GaN, good carrier concentration is accomplished but for p-type concentration of carrier is poor. Mg doped GaN based optoelectronic devices show poor ohmic contacts in metals due to low hole concentration. Mg doped GaN is highly resistive due to the inactivation of Mg acceptors persuade by the formation of Mg-H complexes due to H passivation. The major challenges faced are: threading dislocations density, homo or hetero epitaxy, diffusion of Mg, inactivation of Mg and difficulty in controlling the p-type conductivity. In order to activate the acceptor dopant various techniques are being performed: rapid thermal annealing (RTA) in N_2 atmosphere at high temperatures, low energy electron beam irradiation, microwave treatment, immersion in suitable solvent that breaks Mg-H bond, laser thermal annealing etc.

Keywords: Acceptor, Epitaxy, Conductivity, Annealing

Synthesis of pH Sensitive Hydrogels and their Biomedical Application

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ABSTRACT

A hydrogel is a 3-D polymer network that is water-insoluble and capable of absorbing body fluids while maintaining form and integrity in a biological environment. Stimuli-responsive hydrogels are hydrogels that may change their physical or chemical properties in response to external stimuli. Stimuli include changes in temperature, pH, and light. The synthesis and biomedical applications of pH sensitive hydrogels will be the focus of this paper.

Synthesis of pH-responsive hydrogels involves the use of pH-sensitive polymers such as Poly(acrylic acid) (PAA), Poly(methacrylic acid)PMAA, Chitosan that can swell or de-swell in response to changes in pH . Generally, pH-responsive hydrogels may have a pH range of 3 to 6. It is widely used in drug delivery systems, biosensors, and tissue engineering which undergoes a reversible swelling transition in response to pH changes.

Hydrogels with a high degree of crosslinking may be synthesized using free-radical polymerization, Free radical polymerization is a typical method for creating pH-sensitive hydrogels. The method employs the use of a monomer with acidic or basic functional groups that may be ionised in response to pH variations.

Because of their capacity to adapt to pH changes, pH-sensitive hydrogels have a variety of biomedical applications. Among these applications are;

1. Tissue engineering
2. Biosensors
3. Drug delivery
4. Wound healing

With continued research and development of pH-sensitive hydrogels hold great promise for advancing biomedical and biotechnological applications, and could lead to the development of new and innovative technologies.

PP24

Synthesis and Characterization of Valacyclovir Impurities

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ABSTRACT

An antiviral drug called valacyclovir is used to treat herpes simplex or herpes zoster infections. In high-risk situations, it is also used to avoid cytomegalovirus after a kidney transplant. When active pharmaceutical ingredients (APIs) are created, many impurities or unwanted chemicals emerge from the synthesis that stays with the APIs. These impurities and unwanted chemicals are toxic to the human body and can have a negative impact on health. Both API and formulated APIs in medication may contain these impurities at any time, including during formulation and after aging. The efficacy and safety of drug products can be significantly impacted if unwanted chemicals or impurities, even in trace quantities, are present in API. These could shorten the drug's shelf life and complicate the preparation and use of the substance. Sometimes impurities alter the compounds' chemical and physical characteristics. After a certain amount of time, a drug's therapeutic impact can diminish and it may even start to have toxic effects on the human body. According to a review of the literature, the HPLC technique has identified 17 impurities in the drug Valacyclovir. The literature frequently does not explain the synthesis of impurities, which makes it more challenging for organic chemists who must plan a lengthy synthesis. A drug cannot be developed without an impurity profile being engaged in the process. In the current study, four valacyclovir impurities—named Impurity M, Impurity I, Impurity C, and Impurity H—have been synthesized and characterized.

PU Foam Composite as an Effective Method for Thermal Insulation

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ABSTRACT

Massive amounts of waste are produced during the mass manufacture of polyurethane foam from a variety of items, much of which takes the form of dust that is released during the cutting, trimming, or grinding of the foam. Polyurethane foam (PU) is widely used in building insulation. Waste polyurethane foam (PU) is combined with adhesive to create a thermal insulating composite material that may be used for building walls. The PU foam composite materials were made with compression moulding machine using different ratio of foam and adhesive. In every instance involving composite foams, the polyurethane foam structure was effectively produced whereas, the addition of the natural fibers such as bagasse, sawdust increased the mechanical strength. In order to assess the suitability of the composites for this kind of application, the density, thermal conductivity, mechanical strength of the material were examined. To determine the material's thermal stability, differential scanning calorimeter experiments analysis were used.

Keywords: Polyurethane, foam, composites, thermal insulation, stability.

PP26

Synthesis of Ag/PVA Hydrogels by Gamma Irradiation and its Characterization

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ABSTRACT

Polyvinyl alcohol (PVA) hydrogels are materials which are used in medical research. Silver nanoparticles synthesized within PVA hydrogels possesses high antimicrobial activity. This work developed gamma-irradiated PVA/nano-Ag hydrogels for potential use in antimicrobial applications. Gamma irradiation serves as a crosslinking agent for the polyvinyl alcohol hydrogels and also acts as a reducing agent for the reduction of Ag(I) ions to zero valent Ag (0) within the PVA cross-linked network. Ag NPs are used because of its potential as antimicrobial agent. The formation of Ag nanoparticles in PVA hydrogels is confirmed by using UV-Visible (UV-Vis) spectrophotometer and X-ray diffraction (XRD) studies. The Ag/PVA hydrogels were characterized by swelling degree, Thermal Gravimetric Analysis (TGA), Fourier Transform Infrared (FT-IR), Scanning Electron Microscopy (SEM) and Differential scanning calorimetry (DSC). Antimicrobial action of the encapsulated silver nanoparticles/ hydrogel composite are currently underway in our laboratory.

Keywords: Polyvinyl alcohol, Hydrogel, Silver nanoparticles, Antibacterial activity.

PP27

Flame Retardant UV Curable Coatings for Textile Materials

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ABSTRACT

Ultraviolet curing is a photochemical process in which high-intensity ultraviolet light is used to instantly cure. In this work, UV Curable Formulations are designed by adding monomers, acrylate-based oligomers, phosphorous-based photo initiators and additives. These coating formulations are used to coat textile materials. All liquid formulations become a solid coatings during UV curing. Fourier Transform Infrared Spectroscopy was used to identify the functional groups present in the coatings. By Limiting Oxygen Index and performing a thermo gravimetric analysis of coated textiles the flame retardancy can be determined. Scanning electron microscopy identifies the presences of all additives that are used in coatings. Tensile strength and elongation were used to assess the durability and flexibility of all textiles. Gel content is used to determine cross linking polymerization in coatings.

Application of PVC Membrane based Sensors for Trace Determination of Metal Ions

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ABSTRACT

Determining trace levels of the metal ion is currently the analytical chemists' hardest issue. Due to their distinctive chemical characteristics, metal ions have a wide range of applications in many different sectors. Metal ions are used often in a variety of industries, including electronics, construction, medicine, agriculture, and water treatment. Yet, due to their bioaccumulation in both human and animal systems, the excessive use of these metal ions has not only shown adverse environmental effects but also health hazards. As a result, the problem of quick and accurate metal ion detection has become critical. Metal ion determination can be accomplished using a variety of techniques, including as spectrophotometry, atomic absorption spectrometry, atomic emission spectrometry, electrochemical processes, and spectrofluorimetric methods. Yet, these methods are time-consuming, need for handling several samples, or are prohibitively expensive. An additional technique for the detection of metal ions is the use of potentiometric sensors with polymeric membranes.

Potentiometric sensors are made to pick out and quantify particular ions in solutions. These sensors do have a number of advantages over other instrumental techniques for the detection of trace metal ions, including: Ecologically sound methods, Provides easy building, Displays strong selectivity throughout a wide concentration range of operability, Very low detection limit, rapid response.

In this study, we created a PVC-membrane-based sensor and improved the working conditions for metal ion trace measurement. The same methodology has also been used to identify metal ions in water samples.

Keywords: Metal, PVC-membrane, Sensor, Potentiometric

PP29

Morphological Studies and Applications of Bismuth Oxyhalides Synthesized through Green Route

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ABSTRACT

Due to population development and the quick expansion of industry, worries regarding the elimination of numerous organic poisons are rising and one of the severe poison is dye. The biochemical and chemical oxygen demand (BOD and COD), impairment of photosynthesis, inhibition of plant growth, bioaccumulation, mutagenicity, and carcinogenicity are all considerably compromised by textile dyes. In the process of treating industrial effluents, photocatalysts are essential and are often used in the decolorization of textile dyes. One of the promising methods to increase the photocatalytic activity is to synthesize green photocatalysts for effective separation of photogenerated charges using green route. Recently, a lot of researchers have been focusing on the photocatalytic degradation of dyes using bismuth compounds. The green synthesis of bismuth oxyhalides is done using different plant extracts with good size control, a greater surface area, and porosity and were further tested for photo-degradation of organic pollutants under visible light spectrum range. The as-prepared BiOBr photocatalysts has a two- dimensional (2D) structure with a band gap of 2.87eV. The photocatalytic activities were evaluated by the degradation of Rhodamine B (RhB) under visible light irradiation with wavelength > 420nm and various morphologies are primarily responsible for the variations in the photocatalytic activity.

Keywords: Bismuth oxyhalides; Dyes; Degradation; Photocatalysts; Band gap

Preparation of Low Dimensional (0D and 2D) Transition Metal Dichalcogenides, WS_2, via Simple Chemical Route

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ABSTRACT

Two dimensional ultrathin nanostructures such as transition metal dichalcogenides (TMDs) have attracted wide attention due to their supreme optical and electronic properties. Tungsten disulphide (WS_2) transition metal dichalcogenide, an inorganic compound with stacked layers, has an exceptional nanostructure, wide band gap in the range of 1-2 eV, high surface area, and high charge carrier mobility. These nanomaterials are commonly employed as solid lubricant by various industries. In this study, Tungsten disulphide (WS_2) transition metal dichalcogenide was synthesized by one step hydrothermal approach i.e. without using surfactant for the fabrication of quantum dots & ultrathin film of 2D materials & by corresponding simple, convenient & low-cost technique named, Chemical Bath Deposition (CBD) for large area deposition at high temperature. Synthesised WS_2 transition metal dichalcogenides nanostructures were characterized by using several techniques such as X-Ray Diffraction, UV-Vis Spectroscopy, Photoluminescence, Transmission Electron Microscopy & Raman Spectroscopy. Moreover, synthesised nano-WS_2 product has huge potential in solid lubrication, optoelectronics & gas sensor applications.

Keywords: TMDC, Hydrothermal synthesis, Chemical Bath Deposition, Band gap.

Development of Natural Fibers based Composites using HDPE Polymer

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ABSTRACT

The use of natural fiber as reinforcement in polymeric composites has been established due to environmental concerns and the high cost of synthetic fibers. The present article is focused at to make polyolefin based bio composites containing cellulose fibers particularly hemp as reinforcement and to study its thermal, rheological and mechanical properties. Prior to the composite fabrication TGA, density, MFI, tensile strength, rheological and mechanical tests were employed for the polymer (HDPE) characterization. Cellulose and lignin content of hemp fiber from different sources were tested to get a better knowledge of fiber to be used for further applications.

Composites are being made with the help of kneading and twin screwer and two roll mill. The resultant composite material will be aimed at to manufacture blow molded jerry cans and blue drums. Since HDPE is sensitive to stress cracking and non-biodegradable. Therefore, polymer is reinforced with fiber to make bio composites which is the major concern.

Recent Advances in Synthesis and Applications of Low Dimensional (0D and 2D) Transition Metal Dichalcogenides

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ABSTRACT

Over last two decades, researchers across the globe have minutely investigated 2D transition metal dichalcogenides (TMDCs) due to their unique characteristics in optics, mechanics, electronics, and sensing, which makes them suitable for various electronic and optoelectronic applications. 2D nanostructures of TMDC materials especially have great potential to replace currently used silicon-based technology, or even graphene which is viewed as a possible great substitute. Nanostructures of TMDCs, such as molybdenum disulfide (MoS_2), possess excellent electrical and optical properties, including a favourable direct band-gap of approximately 1.8 eV and high mechanical flexibility. Unlike semi-metallic graphene, MoS_2's semiconducting behaviour enables it to overcome the limitations of zero-band-gap graphene. This study reviews the state of art of various synthesis methodologies for preparing 2D MoS_2 materials, including chemical bath deposition (CBD) and hydrothermal technique. Additionally, detailed characterization protocols and signature features of MoS_2's nanostructures, such as MoS_2 nanosheets, quantum dots, thin films are assembled and explained in detailed manner here. This includes in-depth analysis of such materials using X- Ray Diffraction, UV-Vis Spectroscopy (UV), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Raman Spectroscopy, and Photo Luminescence (PL). This review also compares recent theoretical model-based results with experimental observations to provide additional insights into dielectric, optical, and topological behaviour of MoS_2.

Keywords: Transition metal dichalcogenide, 2D nanostructures, MoS_2 structure and properties

Electroconversion of Biomass-derived Compounds

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ABSTRACT

A novel and promising way to converting biomass into useful chemicals and fuels is electrochemical conversion of biomass. This technique employs electrochemical methods to degrade biomass into its constituent molecules, which are subsequently converted into high-value products. A range of technologies for electrochemical conversion of biomass are available, including electrolysis, electroreduction, and electrooxidation.

The procedure starts with processing of biomass to eliminate contaminants and prepare it for electrochemical conversion. The biomass is then exposed to electrochemical processes, which produce hydrogen gas, biofuels, and other compounds. The primary benefit of electrochemical conversion over traditional biomass conversion methods is that it is a highly efficient and ecologically benign process that does not require combustion. The electrochemical conversion of biomass usually consists of three steps:(I) pre-treatment of the biomass to remove impurities and improve its reactivity, (ii) electrochemical conversion of the biomass into intermediate compounds, and (iii) further processing of the intermediate compounds into final products.

Many electrochemical approaches for biomass conversion have been investigated, including electrolysis, electrocatalysis, and microbial electrochemical systems. Different techniques have distinct benefits and limitations, and their success is dependent on a variety of criteria, including the kind of biomass feedstock, electrode materials, and operating conditions. Biomass electrochemical conversion has the potential to transform the production of chemicals and fuels from renewable resources. It provides a long-term and cost-effective alternative to fossil fuels, which are becoming increasingly limited and expensive. Furthermore, this technique can help to reduce greenhouse gas emissions, so decreasing the effects of climate change.

PP34

Organocatalytic Synthesis of Amides from Amines and Diketones

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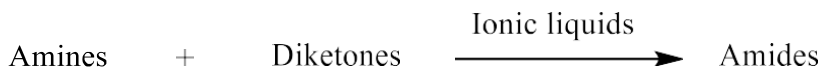
ABSTRACT

We have synthesized ionic liquids using bromo alkanes and imidazole's. Further counter ions were changed to synthesized a series of ionic liquids. These ionic liquids were characterized by ^{1}H NMR and ^{13}C NMR spectroscopic techniques. A metal-free and solvent-free organocatalytic synthesis of amides were demonstrated by the direct reactions of amines and diketones in the presence of ionic liquids. As amides are pervasive in living organisms, which are important structural units in biological proteins and medicinal chemistry. More than 30% of known drugs in the medicinal chemistry analysis database contains amides. In term of industrial synthesis, amides can be used as an intermediate to synthesise polymer nylon which is an important engineering and medical material. Therefore, the synthesis of amides has got much attention in organic synthesis and biochemistry. Earlier, amides have been synthesized in many ways. Most of the reported methods suffer from certain limitations, including the use of transition metals, sensitive starting material, toxic solvents and harsh reaction conditions that's why its highly desirable to develop direct, simple and environmentally friendly methods to synthesized amides. So, we have synthesized amides organocatalytically using ionic liquids. Here, we are focussing on the development of recoverable organocatalysts tailored with imidazolium ionic liquid for organic transformation. An ionic liquid (IL) is a salt in the liquid state whose melting point is below the specific temperature, such as 100°C. So, we synthesized different types of ionic liquids with the help of (1,5-Dibromo pentane) and (N- methylimidazole) and later on, anions exchange reaction was carried out on it. Now, we are focusing on the optimization reaction based on the ionic liquids, anilines, and diketones.

Keywords: Ionic liquids, amines, diketones, amides



Analysing of 6-APA for Synthesis of Amoxicillin

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ABSTRACT

6-Aminopenicillanic acid is very important intermediate for synthesis of antibiotics in pharma industry. The major commercial source of 6APA is still natural penicillin. Industrial approaches to obtain 6-APA include enzymatic as well as chemical route. The present study experimentally is based on the impurities shown in the 6 Aminopenicillanic acid. Impurities are unwanted chemicals in raw material which has to be minimize so that raw material 6APA is further used for the formation of antibiotics such as amoxicillin, ampicillin etc. The presence of these unwanted chemicals can influence the safety of the pharma products. The high number of impurities can cause huge impact in the pharmaceutical industry by lowering shelf life of the substance, may cause complications during formulations as well as can cause heath issues. Furthermore, enzymatic reaction is performed in raw material 6APA to detect the impurities which should not be more than 0.50% to conduct the further formation of antibiotics. The major two peaks of impurities are detected in the raw material 6APA - Phenyl acetic acid and penicillin G potassium.

Keywords: 6APA; impurities; peaks; antibiotics

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Synthesis of Te, N, O Bearing Schiff Base and its Ni(II) Metal Complex for the Study of Structure Driven Inter-/Intra-molecular Interactions and their Employability in Biomedical Applications

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ABSTRACT

We herein report the synthesis of novel bioactive organotellurium substituted Schiff base [(C_6H_3(O)(2-OCH_3){6-HC=N(CH_2)$_3$TePh}] from the condensation of *o*-vanillin and 3- (phenyltellanyl)propan-1-amine in 1:1 molar ratio and its reactivity towards Nickel (II) acetate in 2:1 molar ratio for the formation of functionalized Schiff base metal complex [(C_6H_3(O)(2- OCH_3){6-HC=N(CH_2)$_3$TePh})$_2$Ni]. The synthesized ligand and its complex were fully characterized employing UV-Vis, FTIR, NMR spectroscopy, mass spectrometry, X-ray crystallography, and electrochemical study using cyclic voltammetry. The crystallographic data indicates the crystallization of the complex in P21/n space group in monoclinic fashion and the coordination of Ni(II) metal ion via N2O2 bidentate manner; leaving the tellurium atoms uncoordinated in the system. The crystal also exhibits square planar geometry around the Ni(II) metal ion centre making the N and O atoms of the ligand being *trans* to each other with ∠N1-Ni-N1_a and ∠O2-Ni-O2_a being 180°. Furthermore, Hirshfeld surface calculations were also carried out using the crystallographic information file (.cif) for the study of inter-/intra molecular interactions within the unit cell at hartree-fock level. Moreover, in silico molecular interactions is also studied to explore the biomedical application of the ligand and complex against SARS-CoV-2 (PDB ID: 6M0J) spike protein to discover a potential drug candidate for covid-19.

Keywords: Organotellurium, Schiff base, Ni(II) metal complex, Hirshfeld surface analysis.

Removal of the Reminiscent Dye from the Waste Water by Eco-friendly M TKP-GO Composite

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ABSTRACT

One of the major pollutants in problem of water pollution is the presence of reminiscent dyes present in river and industrial wastewater. It is endangering the world's drinking water sources, and researchers are constantly looking for promising wastewater treatment technologies. Adsorption is recognized as the most convenient approach to low-cost and highly efficient wastewater treatment. Recently, graphene and its composites have been the materials of interest to the researchers as novel adsorbents because of their unique molecular structure and outstanding physicochemical properties. Tamarind kernel powder (TKP) is a natural polymer which is derived from the seeds of the tree Tamarindus indica. It is biodegradable, eco-friendly having low cost. Simple modified hummer's method is used to oxidize the graphite for the synthesis of graphene oxide (GO). Magnetic TKP and Magnetic TKP-GO bio composite were synthesized by the method of co-precipitation. These composites were characterised by FT-IR for their determination of functional groups, XRD was carried out for the study of the crystallographic structure and physical properties. To study the successful and effective incorporation of Fe_3O_4, their size and surface morphology was done by FE-SEM and EDX. The characteristic results of FE-SEM, XRD and FTIR showed that Magnetic TKP-GO was successfully prepared with large surface area and good magnetic response. The given composites were tested for the adsorption of the Congo red dye (CR) from aqueous solution. The influence of various analytical parameters on the adsorption of Congo red such as pH, contact time, and initial concentration were studied in detail. In future this nanomaterial is playing a significant role in solving the challenge of water pollution.

Keywords: Graphene oxide; Tamarind kernel powder; Congo red dye; Wastewater; Adsorption

Use of EDTA and NaCl in Blood Preservation: A Reaction Mechanism of EDTA and NaCl with Calcium

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ABSTRACT

Coagulation, also known as clotting, is the process by which blood transforms from a liquid to a gel, resulting in the formation of a blood clot. It may result in hemostasis, which is the stopping of blood loss from a damaged vessel followed by repair. Platelets (a kind of blood cell) and proteins in plasma (the liquid component of blood) collaborate to stop the bleeding by creating a clot over the damage. Calcium ions (Ca2+) play a major role in the tight regulation of coagulation cascade that is paramount in the maintenance of hemostasis. Ethylenediaminetetraacetic acid (EDTA) is a well-known anticoagulant since early 1950s and it has certain advantages over other anticoagulants. Sodium citrate has been used as an anticoagulant to stabilize blood and blood products for over 100 years, presumably by sequestering Ca(++) ions in vitro. Anticoagulation of blood without chelation can be achieved by inhibition of the contact pathway by corn trypsin inhibitor (CTI). The cascade reactions of Edta and Nacl salt with Blood results in anti-coagulation effect which is indeed important for the sample preservation. In this paper we will study the reaction mechanism and the results for both sodium citrate and EDTA and find which is the best anti-coagulant.

Keywords: EDTA, Chelation, Anticoagulants,Sodium Citrate, Hemostasis.

PP39

Measurements at the Electrode Surface of the Hydroelectric Cell

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ABSTRACT

Hydroelectric cell is a revolutionary green energy source invented by Indian Scientists Dr. Kotnala and Dr. Shah. In hydroelectric cell, processed metal oxide are used to dissociate water at room temperature without the use of any electrolyte or external energy source. Two electrodes zinc sheet and silver conducting paste collect the ions generated from a redox reaction and electricity is produced. The resistance offered by the cell in conducting ions and electrochemical reaction effect the current and voltage performance. The role of resistance at the electrode of Hydroelectric Cell is being studied by measuring and analyzing V-I polarization curve. The data is analyzed to understand the role of resistance at electrode surface in electrochemical reaction to produce voltage and current by Hydroelectric Cell.

Preferential Adsorption Behaviour of Methylene Blue Dye onto the Surface of MPVA-GO Nano-composite

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ABSTRACT

World is facing acute problem of the scarcity of the sources of drinking water. Release of substances, such as chemicals and heavy metals occur due to draining of agricultural and industrial wastewater, resulting in water pollution. These contaminants interfere with the beneficial uses of the water or with the natural functioning of ecosystems. These unsustainable interferences have is attracted a huge attention of researchers for the remediation of the pollutants. Many methodologies are being used, among which adsorption is one of the most popular methods. Poly vinyl acetate is a low cost, readily available versatile adsorbent. It is non-toxic and can be readily degraded by micro-organisms. Graphene oxide is an oxidised form of graphite and is a chemically modified graphene containing oxygen functional groups such as epoxides, alcohols, and carboxylic acids. Synthesis of nano composite of magnetic polyvinyl acetate (MPVA) and MPVA- GO were carried out by the method of co-precipitation. These composites were characterised by FT-IR for the determination of functional groups. XRD study of the crystallographic structure and physical properties of MPVA-GO was carried out to examine the adsorption behaviour. Efficacious incorporation of Fe_3O_4, their size and surface morphology were characterised by FESEM and EDX. The impact of the parameters such as temperature, pH, time of contact and concentration of dye solution in affecting their behaviour of Methylene blue dye absorption in aqueous medium was observed for finding the optimum parameters for highest adsorption. Results concluded that the prepared composites could be used as eco-friendly, stable, and efficient adsorbents for methylene blue dye in wastewater treatment.

Keywords: *Graphene oxide; Polyvinyl Acetate; Methylene Blue; Wastewater; Adsorption.*

PP41

Usage of Biomaterial Polymers in Radiotherapy

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ABSTRACT

Radiation therapy plays an important role in the treatment of cancers. It is the most used technique with different set modalities. After the introduction of radiotherapy in the field of cancer treatment there is significant change and improvement that has happened in the treatment as well as in the planning. The variations occur in the treatment delivery modalities as well as in the dose deposition and in the QA or in QC of the materials. There has been a drastic change in the use of the materials in the past and present studies.

Now days people are shifting towards more effective, eco-friendly, cheaper biodegradable and renewable biomaterials which gives better results than the previously used artificial materials. These Biomaterial polymers can be natural or synthetic. Nowadays in medical sciences there is significant advancement and widespread use of material made of synthetic polymers which is then used in the manufacture of the radiotherapy tracers, brachytherapy sources, 3D printed bolus, fiducial markings, test tools, quality assurance tools, and in the tissue equivalent phantoms. Recent studies have found that organic or naturally occurring polymers have more tissue equivalent properties and give better results in the dosimetry than the artificially synthesized polymers. The polymers which are used in radiotherapy are polyvinylchloride (PVC), polyethylene (PE), polypropylene (PP) and also some biopolymers which are being extracted from living organisms like plants, animals, fungi, microbes starch, cellulose, alginate, agar, chitin/chitosan, hyaluronic acid, xanthan, dextran, silk, collagen/gelatin, elastin, polyaminoacids, polylactic acid, natural rubber, shellac and Rhizophora spp., DSF (defatted soy flour)[3]. One of the latest studies used Rhizophora spp. in the production of the tissue equivalent phantom and it is found that these biomaterials are better than any of the material that has been used so far. In our study we will discuss about the biomaterials which are being synthesized using natural polymers.

Keywords: Polymers, Biomaterials, Radiation Therapy, Cancer

PP42

Organocatalysis for the Asymmetric Michael Addition of Cycloketones and α,β-Unsaturated Nitroalkenes

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ABSTRACT

Michael addition is one of the most important carbon-carbon bond formation reactions in which conjugate addition of enolate ion to α, β unsaturated carbonyl compound in the presence of base will take place. Recently we use thiourea organocatalyst instead of metal catalyst because they are less expensive and create very less environmental problems. In this study, (R,R)-1,2-diphenylethylenediamine (DPEN)-based thiourea organocatalyst was applied to the asymmetric Michael addition of Nitroalkenes and Cycloketones to produce a chiral product. The reaction proceeded with a relatively high level of enantioselectivity achieved using double activation through the hydrogen bonding of the nitro group and thiourea. Product formed were highly enantioselective and diastereoselective. There yields are varying in the wide rang of 88-99% depends upon different types of ketones used. This catalyst used are recovered after the reaction. Resultant compound was analysed with the help of characterization techniques like ^{1}H NMR,^{13}C NMR, HPLC, FT-IR, GAS CHROMATOGRAPHY, MASS SPECTRA, DFT Calculation. This method is based on green chemistry principle because in this we use water as a solvent.

Synthesis of Smart Polymers for Drug Delivery in the Treatment of Cancer

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ABSTRACT

The term smart polymer embraces a wide range of different compounds that can change their color, transparency or shape in response to their environment. Smart polymers are of great interest for drug delivery systems where they can be used to control the release of drugs until they have reached their desired destination. Some of the stimuli to which the polymeric drug delivery systems are responsive are temperature, pH, light as well as some are bio-responsive. Various types of polymers have been used for drug delivery process. Some of them are polypropylene, polyethene, Teflon etc. Polymeric carriers have the ability to load multiple drugs simultaneously and can increase drug concentrations by penetrating the target tissue. They can be used to reduce the steps of chemotherapy. Many cancer drugs varied side effects that can cause a lot of damage to healthy cells, but with the use of polymer-carriers, the side effects of the drug are minimized, this is due to the delivery of the drug to the target tissue, which prevents the drug from affecting other cells.

Keywords: Smart polymers, Stimuli, Cancer, drug delivery

Determination of Trace Amount of Metal Ions using PVC based Potentiometric Ion Selective Electrode

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ABSTRACT

Most of the analytical chemists, nowadays are facing challenge in determining the trace amounts of metal ions. Such amount of metal ions should be determined as they play significant role at chemical, biological and as well as molecular levels. Metals such as nickel, platinum and paladium are used in various industries as catalysts. Copper, gold and silver are used in the production of various electronic components such as wires, computer chips and printed circuit board. Lithium and cobalt are used in the production of batteries for electric vehicles and renewable energy storage systems. Iron, zinc and copper are used in the production of medicines and supplements to treat various medical conditions.

However, overuse of metal ions could be toxic for the environment. Metals such as cadmium, chromium, and nickel can detriorate the quality of soil and water, making them hazardous to biotic life. It is therefore necessary to determine the accurate amount of metal ions. There are various analytical techniques for the determination of trace amounts of metal ions including spectrophotometery, atomic absorption spectrometery, atomic emission spectrometery, electrochemical methods, and spectrofluorometric methods. These methods proves to be expensive, time consuming and involves multiple sample manipulation. Potentiometric ion selective electrodes hence proved to be an effective method for the determination of trace amount of metal ions as these method are simple, fast, inexpensive and shows response over a broad concentration range. The ionophore based potentiometric sensors, used for determination of ions, are called ion selective electrodes (ISEs). ISEs bind the ions of interest at various concentration ranges. Important parameters of ISEs includes detection limit, response time and lifetime, working concentration range and pH . In the present work, PVC based ISE is synthesized using fixed ratio of polyvinyl chloride (PVC), plasticizer, electroactive species called ionophore and lipophillic additive and are used in the analysis of various environmental samples.

Keywords: PVC-membrane, trace, potentiometric, spectrometry

Adsorptive Removal and Photocatalytic Degradation of Methylene Red Dye using the Composites of BiOBr@SiO2

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ABSTRACT

The most vital resources, water is being polluted by industrial waste. Industrial dyes, which kills aquatic life due to a lack of oxygen and disrupts the food chain. As a result, it is impossible for us to access safe drinking water. Nanoscale semiconductor photocatalysts have drawn increasing attention because of their high surface to volume ratio, where dye absorption would be substantial. In this work, we will compare biologically synthesised SiO_2 made from coconut husk and composite of SiO_2 with BiOBr, which was also made from a biological source, degrade the methylene dye. The composite of SiO_2 boosted visible light absorption, it demonstrated better photocatalytic activity than silica alone. Structure as well as properties of the material are studied using various techniques like Ultraviolet spectroscopy (U.V), Scanning electron microscopy (SEM), Fourier Transformer IR (FTIR) Spectroscopy, Dynamic Light Scattering (DLS).

Keywords: silica, bismuth oxy bromide, facile synthesis, degradation of dye, methylene red dye.

Effect of Doping Metal on Electrical and Optical Properties of Semiconductor Nanocrystal Quantum Dot

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ABSTRACT

In this work, by using density functional theory (DFT)-based calculations, we will clearly demonstrate that the incorporation of some metal dopants like Cu, Ag, Mn etc. into the surface and the core of the Cd33Se33 QD leads to the change in it's electrical and optical property. In materials such as CdSe NCs, a model system for studying the electronic and photophysical properties of doped II-VI semiconductor NCs, there is still disagreement on the oxidation state of metal ion whether it presents a +1 or +2 valence state. In this work we will also study the effects of the oxidation state of metal ion on the semiconductor nano crystal.

We would like to address to the following questions:

While doping how many atoms can be doped into the semiconductor?

Which site, whether surface or core of the nanocrystal, is best for doping?

After doping how much efficiency of the semiconductor QD has been increased?

What are the various applications of this doped semiconductor quantum dot?

Psychedelic drugs, Anesthesia and Human Consciousness: A Review

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ABSTRACT

Consciousness refers to the inner subjective first-person perspective experience we have of the world around us. In simpler terms, consciousness is the ability of complex biological systems to feel, sense, or be aware of the world around them. Consciousness emerges from neuronal activity in the cortex of the brain. Several chemical compounds like drugs, anesthesia, and neurotransmitters seem to affect conscious awareness. Psychedelics are a category of non-addictive psychoactive hallucinogenic drugs having immense potential to cure mental illnesses like anxiety, depression, post-traumatic stress disorder, etc. These drugs have been hailed as a boon for psychiatry. However, the interaction of these drugs with receptors in the brain is a matter of open discussion. These drugs are reported to trigger an expansion of consciousness. On the other hand, general anesthesia is used during surgeries to induce loss of consciousness. Most of the general anesthetic gas inhalants are chemically non-reactive and have diverse chemical structures. Psychedelics and anesthesia elicit opposite effects in the brain. Present review work borrows ideas from orchestrated objective reduction theory of consciousness, first proposed by Sir Roger Penrose and Stuart Hameroff in the 1990s. It highlights the role of quantum effects taking place in sub-cellular cytoskeletal organelles called microtubules in neuronal activation. It also sheds light on the mechanism of interaction of psychedelic and anesthetic substances in the neuronal cytoskeleton and the accompanying changes induced in the state of consciousness.

Keywords: Psychedelics, microtubules, objective reduction, anesthesia, consciousness

Microwave-induced Grafting of Acrylonitrile onto Rayon Fiber for Biological Applications

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ABSTRACT

Rayon is a semi-synthetic fiber with light weight, breathable, and moisture absorbent properties. Acrylonitrile (AN) is used as a grafting monomer to further increase the swelling capacity of rayon. In the present work acrylonitrile grafted rayon (AN-g-Ry), is synthesised for designing a new material which may be used for biological applications. Graft copolymerization is used as a versatile technique to prepare AN-g-R so as to modify its physico-chemical characteristics influencing the swelling behavior, wettability, antimicrobial properties etc. AN-g-Ry is optimized for various parameters including amount of monomer, initiator, temperature and reaction time of grafting etc. and is further morphologically and structural characterized through IR spectroscopy, XRD spectroscopy, SEM techniques. Swelling characteristics of AN-g-Ry shows its potential properties for biological applications.

Keywords: Rayon fiber, acrylonitrile, Grafting, swelling capacity

2-D Material Based Wearable Biosensors: Fabrication Strategies, Challenges and Future Scope

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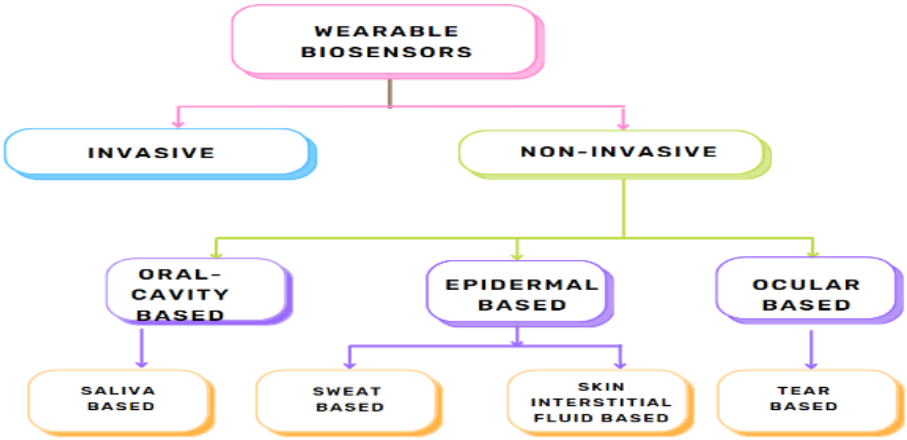
ABSTRACT

Wearable biosensor systems, which can track vital signs in real-time and quantify human health information, have been intensively researched as an evolutionary triumph in the field of life science. The creation of sensors using a variety of flexible materials is the primary area of research for wearable biosensor devices. Current wearable technology is primarily made of soft silicon and organic polymers and often takes the shape of tiny blocks of wireless flexible electronic/sensing components. Both materials, however, have significant limitations. For example, wearable systems based on silicon have difficulty maintaining device performance under severe strain conditions, whereas wearable devices based on organic polymers have limited device performance because of their low carrier mobility. Research has been focused on developing new two-dimensional (2D) materials to replace silicon and conductive polymers, which are the traditional solutions to these problems. Among these, 2D materials with excellent flexibility and mechanical properties, large surface area, low sheet resistance, high carrier mobility, and high biocompatibility offer the anticipated qualities to overcome the difficulties of creating microminiaturized wearable biosensor devices. In this poster, current applications in biosensing technology, such as electronic skins, contact lenses, oral sensors, glove sensors, acoustic sensors, and man-machine control systems, based on 2D materials, such as graphene, transition metal dichalcogenides (TMDCs), black phosphorus, and transition-metal carbides (MXenes) have been discussed. Also, it includes the most recent developments in biosensor systems involving wearable wristbands, diabetes patches, and intelligent contact lenses.



Keywords: *2-D materials, Biosensors, wearable sensor*

Modern Approaches in the Synthesis of Optically Stimulated Luminescent (OSL) Materials for Dosimetry Applications

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ABSTRACT

Optically stimulated luminescent (OSL) materials have become increasingly important in the field of dosimetry. They are widely used in various applications, including radiation therapy, environmental monitoring, and personal dosimetry. OSL materials have several advantages over traditional dosimeters, including high sensitivity, high spatial resolution, and high accuracy. As a result, there has been a great deal of interest in developing new approaches to synthesize OSL materials. Modern approaches to the synthesis of OSL materials for dosimetry applications include various techniques such as sol-gel method, hydrothermal synthesis, microwave-assisted synthesis, and chemical vapor deposition. Among these techniques, sol- gel method has been extensively used for the preparation of OSL materials. This technique involves the hydrolysis and condensation of metal alkoxides to form a gel that can be converted into a solid material by heating. The sol-gel method has several advantages over other techniques, including its ability to produce materials with controlled particle size and morphology. Another promising approach for the synthesis of OSL materials is hydrothermal synthesis. This technique involves the use of high-pressure, high-temperature water to promote the formation of crystalline materials. Hydrothermal synthesis has been shown to produce high- quality OSL materials with high luminescence efficiency and excellent dosimetric properties. Microwave-assisted synthesis is another approach that has gained attention in recent years. This technique involves the use of microwaves to promote the rapid and efficient synthesis of OSL materials. Microwave-assisted synthesis has been shown to produce high-quality materials with excellent luminescent properties. Chemical vapor deposition (CVD) is another technique that has been used for the synthesis of OSL materials. This technique involves the deposition of thin films of material onto a substrate using a gas-phase reaction. CVD has several advantages over other techniques, including its ability to produce high-quality films with excellent control over thickness and composition.

In the present review article, we will discuss in detail about the modern approaches of synthesis of OSL materials for dosimetric applications.

Utilization of Carbon Dioxide via Cycloaddition with Epoxides using Green Catalysts

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ABSTRACT

The carbon dioxide is being released in the atmosphere through fossil fuel burning, and auto-mobile activities and thereby high concentration of this greenhouse gas causes global heating across the world. The atmospheric carbon dioxide being inexhaustible, low-budget, and a sustainable resource is captured and utilized as building blocks for the synthesis of many useful organic compounds. Herein, we focus on the synthesis of cyclic carbonates from epoxide and carbon dioxide as reactants. Cyclic carbonates being versatile compounds are synthesized by cycloaddition of carbon dioxide with epoxide. The applications of cyclic carbonates vary from electrolytes in batteries, polymer precursors, fuel additives and to an aprotic high-boiling point solvent. Heterogeneous catalysts such as Metal-Organic Frameworks (MOFs) and Ionic Liquids are being used as catalysts in cycloaddition reaction. Their catalytic activity along with the reaction conditions, and selectivity were analysed and compared. Reducing the superfluous carbon-dioxide emissions and transmogrified them into sustainable products is one of the attributes of green approach. Both catalysts exhibit a high catalytic activity for the cycloaddition of carbon dioxide.

Analysis of the Partial Pressure of Hydrogen Gas using CH-II Mission Data

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ABSTRACT

The variation of the partial pressure of the hydrogen gas in the space over the course of a year was studied using the data that was retrieved by the Chandrayaan-II payloads during the successful term of the mission. Monthly based analysis was done using the payload data and it was found that, in interstellar space, the partial pressure of hydrogen gas is much higher. It was found that partial pressure varies as a result of seasonal changes in the atmosphere of the planet, for example in the winter months the partial pressure is an average of 2.92 Pa for the month of January whereas it is 4.56 Pa for the month of February. Similarly in the summer season, the partial pressure reaches to an average of 0.10 Pa in the month of June and in the month of August the average reaches out to 0.046 Pa. However, for the Spring Summer season, the average partial pressure in the month of March was 19.37 Pa, which is high when compared to the previous month, whereas in the month of May the average decreases to 0.14 Pa. Now looking at Autumn season, it was found that the average partial pressure was recorded as 6.74 Pa for September month, 14.02 Pa for the month of October and 19.55 for the month of November. The above investigations, thereby provide a proper variation of the partial pressure for all the months of the year corresponding to the seasonal changes that occur throughout the year.

Keywords: Hydrogens gas, Paylaod, Chandrayaan-II, Partial pressure

PP53

Photocatalytic Hydrogenation of CO_2 over Bi-based Photocatalyst

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ABSTRACT

Photocatalysis based on semiconductors/catalysts has recently sparked significant scientific interest due to its numerous applications in environmental beneficiaries and renewable energy generation. Considering this, knowledge of photocatalyst selection, and catalytic regulation, Furthermore, adjusting the band gap improves the target hydrocarbon product's yield, specificity, and selectivity. To better match, a photocatalyst for improved CO2 capture and conversion into specific hydrocarbon fuels, several insights about the best way have been offered to tune a photocatalyst. Course of the most recent but not least, the current situation, difficulties, and prospects for producing photocatalysts with higher Carbon dioxide reduction effectiveness and significant product yield is reviewed. Bismuth-based compounds have the potential to be photocatalytic materials for moderate and long-term CO2 conversion. Catalysts were made using a simple deposition, precipitation, and solution process. The objective of this review is to provide in-depth systematic information on different photocatalysts that have been used over the years and discuss factors that influence their effectiveness. The discussion covers a range of modification techniques for fine-tuning the characteristics and enhancing photocatalyst performance. Composites or heterostructures developed with these modification approaches are also evaluated. Efficiency comparisons of active compounds or heterostructures with TiO_2 are provided in this overview, followed by useful, practical advice and recommendations for further development.

Characterisation of Chemical Mass and Metallicity of Different Stars using Computational Tools (Mesa and Madstar)

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ABSTRACT

Stellar evolution is a complex process that involves many physical phenomena, such as nuclear fusion, radiation, and convection. Studying these processes requires sophisticated computer simulations, which are often computationally intensive and require specialized software. Online tools such as MADSTAR, NAAP, and MESA help to make these simulations more accessible to students and researchers alike. In this study, we utilized these online tools to simulate the evolution of stars with different masses and initial conditions. MADSTAR for simulating the early stages of star formation, including the collapse of a cloud of gas and dust into a proto-star. This study demonstrates the power of online tools for simulating complex physical processes and provides insights into the complex evolution of stars These tools have the potential to make the study of astrophysics more accessible and engaging for students and researchers alike.

Keywords: metallicity, stars, computational tools

PP55

Understanding Protein Misfolding Diseases and Its Potential Therapeutic Strategies

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ABSTRACT

Proteins play a pivotal role in various biochemical processes in our body. However, certain irregularities in protein folding and formation of its aggregates paves the way to a plethora of debilitating diseases such as Alzheimer's Disease (AD), Parkinson's Disease (PD), Huntington Disease (HD), Amyotrophic Lateral Sclerosis (ALS), Type-II Diabetes, etc. The rapid increase in the number of people suffering from these diseases across the globe and the lack of complete cure has resulted in a lot of attention in this research area. Proteins take up their functional tertiary or quaternary form by folding up in an intricate way such that the hydrophobic parts are buried in the interior regions of the structure. Cellular stress or mutations cause these hydrophobic portions to be exposed to the exterior region which then interact with each other causing misfolding. These could then form aggregates or amyloid plaques which disrupts cell function and could be toxic causing cell death. We will try to understand the factors controlling the proper protein folding, causes of disruption of protein homeostasis leading to toxic irregularities and various potential therapeutic strategies to combat the protein misfolding diseases. In particular, we will discuss about the chaperone based therapeutic approach for these diseases.

PP56

Silver Nanoparticle: Synthesis, Catalytic Activity and Other Application

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ABSTRACT

Silver nanoparticles are synthesized by traditional route in lab, but they suffer from an unavoidable drawback that they are highly toxic in nature. Therefore, AgNPs are placed on a solid support for diverse application in the field of biological, electronic, optical and catalytic properties. These exhibit great stability, high reactivity, very selective and efficient, which makes them favorable catalyst. Many AgNPs like supporter on LDH are stable, reusable and ecofriendly. They are dispersed on the surface of a solid support by hydrogen bond between carboxylate group of reactant and hydroxy group. It was discovered that catalytic oxidation property of silver nanoparticle is significantly influenced by the crystal faces of the AgNPs. Silver nanoparticle also having other application means that sliver having a strong toxicity towards many microorganisms. Silver having antimicrobial properties. Silver used in commercially product in which it acts as a preservative, silver thiosulfate complex is present in packaging plastics for long- lasting and provided antibacterial protection. AgNPs with different nanocomposite materials have been obtained in polymeric resins, polymeric membrane and in fibers. There are several synthetic routes for preparing AgNPs using the currently available technology including electrochemical method, vapor deposition method and some other processes.

Recent Advances in the Synthesis of Thermoluminescent Materials for Dosimetry Applications

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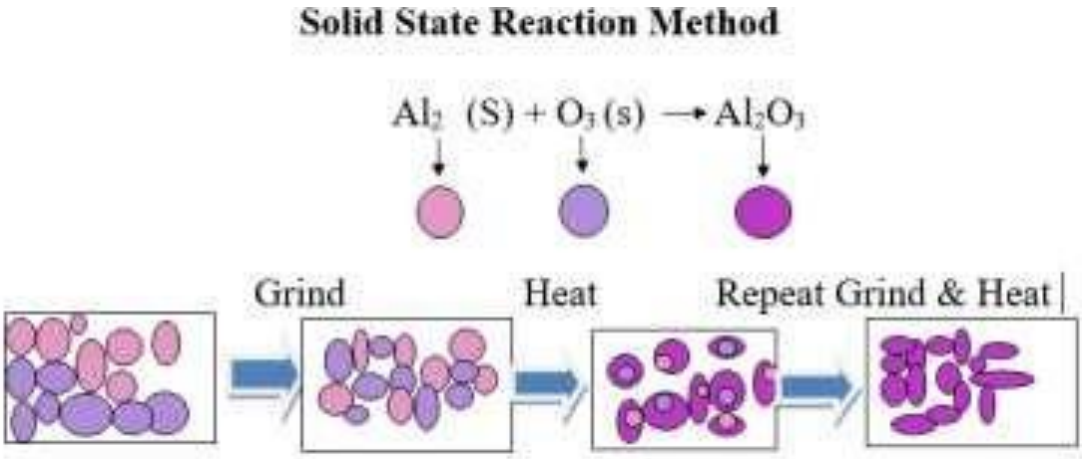
ABSTRACT

Due to their potential use in a number of areas, such as radiation dosimetry, medical imaging, and environmental monitoring, thermoluminescent materials have attracted a lot of attention. The creation of materials with improved thermoluminescent qualities, such as higher sensitivity, high radiation response, and stability, has been made possible by the development of novel synthesis pathways and processes. Sol-gel, co-precipitation, and hydrothermal synthesis have all been used to create diverse kinds of thermoluminescent materials, including inorganic chemicals, organic compounds, and nanomaterials [1, 2]. Understanding the structure and characteristics of these materials has been aided by the application of cutting-edge characterization techniques like X-ray diffraction, scanning electron microscopy, and thermogravimetric analysis. The synthesis of thermoluminescent materials has enormous potential for enhancing radiation detection and monitoring, and continuing studies in this area continue to propel developments in the sector. In this paper, we shall talk about various thermoluminescent materials' synthesis processes.



Ultrathin Solar Cells: Challenges and Recent Research

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ABSTRACT

Ultrathin solar cells, which have a thickness of about 10µm and are about 10 times thinner than standard solar cells, have many advantages over the former. The range of their benefits is quite broad, from improving light trapping efficiency and conversion efficiency to being cost-effective. Yet, there are obstacles when it comes to the implementation of this kind of technology. We will explore methods to ensure effective charge collection while addressing difficulties in the manufacture of incredibly thin absorber layers and in the nanoscale patterning of light-trapping structures. Finally, we highlight future research areas and potential applications of ultrathin photovoltaic technologies, as well as viable topologies for ultrathin solar cells that integrate photonic and electrical restrictions. Lastly,a brief introduction on ultrathin organic solar cells and their future aspects.

Utilization of Brine Sludge in Making of False Ceiling

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ABSTRACT

Significant amounts of brine sludge (BS), which is frequently disposed in industrial landfills, are produced by the chlor-alkali industry. Many chemical components of BS have a negative impact on the environment. A feasible study was done to see whether brine sludge wastes might be utilised to make value – added products. The elements recognized in the sample were Ca, Si, Na, Mg, Al, Cl, and Fe. The main components of the brine sludge samples were quarts, magnesium hydroxide, calcium carbonate, and salt chloride. In this study the Brine sludge was used in making of false ceiling and its properties were evaluated.

Keywords: Brine sludge, false ceiling, concrete, flexural strength.

PP60

Anticancer and Antimicrobial Studies of Stannane of D Biotin

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ABSTRACT

The goal of this research was to develop an effective drug that could act as an anticancer and antimicrobial agent. A constant method was used to synthesize D-biotin stannane in a benzene-ethanol medium by azeotropically removing water molecules from the reaction system.

It was initially subjected to a Dean-Stark fixture at reflux followed by a rotor-vacuum evaporator to remove residual solvent from the system and characterized by spectral analysis (1H NMR and FTIR studies). The in vitro antibacterial study of the complex was carried out against Bacillus subtilis MTCC121 (gram positive) and Pseudomonas aeruginosa 1934 (gram negative) bacterial strains by the "bond diffusion method". The experimental results were further compared with the control (chloramphenicol) after 24 hours of incubation.The synthesized complex inhibited the growth of Bacillus subtilis MTCC121 (gram positive) and Pseudomonas aeruginosa 1934 (gram negative) bacteria in an in vitro antibacterial study. In silico docking studies were performed using the iGemDock v2.1 tool of the computer software and its interaction with PDB 1 m14 (epidermal growth factor receptor tyrosine kinase domain) was studied. In an insilico study, an amino acid in the tyrosine kinase domain of EGFR showed effective binding to the synthesized complex and prevented the overexpression of the epidermal growth factor receptor (EGFR), which causes various cancers such as breast, lung, ovarian, and prostate cancer. The result indicated that the complex could be used to prevent protein dimerization and therefore exert chemotherapeutic effects on the epidermal growth factor receptor tyrosine kinase domain. Thus, the new complex was found to be a good anticancer agent.

Keywords: Stannane, Insilco and In vitro antibacterial study, Computational Chemistry, Anticancer agent, Protein Data Bank files (PDB), EGFR.

Modern Approaches of the Synthesis of Chemicals used in Dosimetry

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ABSTRACT

Chemical dosimetry is simply a method or system created to gauge the amount of energy absorbed by ionising radiation during irradiation. Every chemical dosimeter produces at least one new species as a result of chemical interactions, and this new species has characteristics that let us assess its quantity or the degree of change in the starting systems. It can be found in many different forms, including as solid, liquid/aqueous, and gaseous. Due of their processing and production capabilities, aqueous systems are frequently utilised in radiation facilities. Chemical dosimetry dates back to the Golden Age, when pastilles, iodine compounds, and chloroform-based chemical dosimeters were first developed. Despite the fact that there are many different chemical dosimeters available today, currently, we use Fricke, ceric cerous, and alanine dosimeters the most for chemical dosimetry. In this paper, we will go through how different chemicals are synthesised for usage in dosimetry applications, as well as how "Fricke" and "alanine" dosimeters are made and configured.

Recent Advances in Chemical Dosimetry and its Application in Small Field Dosimetry in Radiotherapy

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ABSTRACT

Radiation dosimetry is a wide topic that includes all three domains of science, physics, chemistry, and biology. With the course of advancement in research and technology and demand for alternatives in dosimetry applications, chemical dosimetry is striving its path to replace the established ionization and film-based dosimetry protocols. Several research are in progress in initiating dosimetric procedures based on radiation induced polymerization of gel and amino acid-based alanine chemicals which basically depend upon the quantification of absorbed dose based on the chemical change occurring in materials when exposed to ionizing radiation. Currently used chemical dosimeters have the capability of quantifying the dose distribution in 3D and have wide dose range, 3D mapping and reproducibility characteristics which increase their potential to be used in radiotherapy dosimetric applications, especially in small field dosimetry, being practised in 3D highly conformal therapy and advanced stereotactic radiation therapy applications. These dosimeters help in overcoming the dosimetric uncertainties created due to the limitations of detector based small field dosimetry, and it is certain that chemical dosimeters are proving to be a great alternative for the existing ionization chamber and film-based dosimetry protocols used in radiotherapy.

In this article we will be discussing the recent advances in chemical dosimetry and its application in small field dosimetry in the field of radiation oncology.

PP63

Advances of Radiochromic Films used in Radiotherapy

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ABSTRACT

Radiation dosimetry Is the fundamental requirement procedure performed for the determination of exposure from ionizing radiation which is utilized in treatment of cancer patients.

Ionization chambers, semiconductors, thermos luminescent detectors (TLDs), and radiographic films are being used in the field of Radiation oncology for the evaluation of dose distributions with high-gradient beams using traditional measuring techniques, though these techniques posed certain limitations and constraints which resulted in uncertainties in dosimetric measurements, which led to the introduction of "radiation induced polymerization" based radiochromic film dosimetry Radiochromic films have found to provide increased output accuracy with less energy and atmospheric dependence.

The organic polymers polyvinyl chloride (PVC), polyvinyl alcohol (PVA), and polyethylene terephthalate are predominantly used in radiochromic film coatings as these polymers are renowned for their high radiation sensitivity and radiation stability. Dyes like Malachite Green, Bromophenol Blue, and Bromocresol Purple are being used to increase the sensitivity and clarity of PVA and PET materials.

Inorganic polymers like lithium fluoride (LiF) are also being utilized additionally as radiochromic film coatings due to their high radiation sensitivity and minimal background noise,

Recent advanced radiochromic materials in use are plastic gels, chitosan-gelatin films, poly (ethylene glycol) diacrylate (PEGDA), 2-hydroxyethyl methacrylate (HEMA), etc. The development of radiochromic film materials continues to be a major field of research. More research can be done with monomers like polyvinyl chloride (PVC), polyvinyl alcohol (PVA), and polyethylene terephthalate (PET)which are sensitive to radiation and have great affinity to get polymerized after radiation treatment. Several methods for developing low or no-diffusion materials enabling radiochromic systems to be used with different polymerization materials for many high-dosage gradient outputs are in progress and it is certain that future advancements in the field of polymer-based radiochromic film optimization would pave way for improved radiation therapy and diagnostic dosimetric procedures.

Keywords: radiochromic Films, Polymerization, Radiation-Induced polymerization

Advanced Materials and their Suitability for Catheters and Applicators used in Brachytherapy

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ABSTRACT

In Brachytherapy radioactive sources - are placed right into the tumour or in its immediate vicinity. In order to ensure that the tumour receives the required radiation dose while minimising exposure to the surrounding healthy tissues, the sources are guided and positioned to target site within the body using catheters and applicators. These catheters must be made of materials that are biocompatible, and non-toxic to the patient and environment friendly. Hence, selection of suitable material for catheters and applicators for medical treatments is essential and discussed in the study.

Brachytherapy success is greatly influenced by the materials that are selected for manufacturing Catheters and applicators'. They must be sterile, flexible, strong, long-lasting, biocompatible, cost effective and environment friendly. The study talks about the unique qualities of silicone, polyurethane, and other advanced materials which are being explored and tested for their suitability at different parameters for manufacturing catheters and applicators in brachytherapy. The most popular materials available in market for brachytherapy catheters and applicators are silicone, polyurethane, and nylon. Polyurethane is used for its hardness and shape-maintenance properties, whereas silicone is chosen for its flexibility and nylon for its strength and longevity.

The limitations behind selection of suitable materials in catheters and applicators are also covered in the paper. The risk of adverse responses and problems in patients can be significantly decreased by ensuring biocompatibility and non-toxicity parameters. The review highlights the importance of choosing the best material for the catheters and applicators in order to ensure their maximum safety and effectiveness during medical procedures. It also provides insightful information about the advanced materials used to make catheters and applicators for brachytherapy and the factors that play a crucial role in their selection.

Keywords: Brachytherapy, Catheters, Applicators, Materials, Biocompatibility.

Smart Sustainable Solutions to Mitigate Water Pollution in Yamuna River

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ABSTRACT

The condition of the Yamuna River in the National Capital Territory presents a grim picture. The quality of water not only raises serious health concerns but also jeopardizes the biodiversity and aquatic ecosystems in its vicinity. Throughout the 48 km stretch of Yamuna along the NCT (from Palla village to Okhla bridge), it receives millions of gallons of sewage/wastewater. In addition to this, the discharge of untreated industrial effluents causes alarmingly high levels of ammonia, heavy metals like chromium (Cr), nickel (Ni), copper (Cu), zinc (Zn), arsenic (As), cadmium (Cd), lead (Pb) and mercury (Hg), dyes, pesticides etc. [3]. Various initiatives have been taken by the government to improve the quality of water in Yamuna River. The Yamuna Action Plan is one of the largest restoration projects in which billions of money spend to combat the situation. The present work discusses the major contributors of wastewater (treated/untreated), discharged in the Yamuna River. The timeline of various initiatives taken by the government to mitigate the pollution levels in the river is discussed. The working methodology for the water sample testing at different locations of river Yamuna is presented. The interpretation of test results to design a robust base for further course of action is also mentioned. The novel sustainable approaches to combat the current problem by reinforcing the Yamuna cleansing initiatives are also proposed.

Keywords: Yamuna, sustainable, wastewater, ecosystem

Synthesis of Magnetically Recoverable Zeolite from Industrial Wastes

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ABSTRACT

Magnetic zeolites were synthesised by hydrothermal activation at low temperatures in an environmentally conscious manner. The novel aspect of the procedure is the use of a mixture of industrial waste products (fly ash (FA) and red mud (RM)) as precursors for the one-step synthesis of high-quality magnetic zeolite. Production of zeolite from industrial wastes like fly ash and red mud are considered to be one of the most promising environment friendly sustainable solution. crystallinity, particle characterised using SEM (Scanning Electron Microscopy), XRD (X-Ray Diffraction) and EDAX (Energy Dispersive X-Ray Analysis) for identification and determination of properties like crystallinity, particle size and morphology. The synthesised zeolite was used for the removal of chromium from water. The prepared zeolite was found to possess magnetic property and could be easily removed from the system using an external magnet. Due to their ease of separation by an external magnetic field, magnetic zeolite was considered to be good alternative for water treatment.

Efficient, Targeted Drug Delivery Using Nanomaterial based Carriers

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ABSTRACT

Targeted delivery of medicinal drugs to diseased cells in body is one of the most significant areas of pharmaceutical research. Nanomaterials with ultrahigh surface area, good aqueous solubility and facile functionalization capabilities have proven to be an ideal platform for loading and delivery of drug molecules. These nano size materials can be easily designed to deliver drugs to specific targets in the body, such as tumour cells, while minimizing damage to healthy cells. Small size of nanoparticles allows for more precise targeting of cells or tissues, which can increase drug efficacy and reduce side effects. Secondly, nanoparticles can protect drugs from degradation and clearance by the body's immune system, allowing for longer circulation times and increased drug availability. Additionally, nanoparticles can be engineered to release drugs in a controlled manner, allowing for sustained drug delivery over time. Nanoparticle based drug delivery system has been used in a variety of applications, including cancer treatment, gene therapy, and vaccine development. However, there are still challenges to overcome, such as the potential toxicity of nanoparticles and the difficulty of scaling up production. Despite these challenges, the field of nanoparticles drug delivery continues to advance and holds great promise for improving the efficacy and safety of drug delivery in the future.

Keywords: Drug delivery, Nanomaterials synthesis and functionalization, Cell cytotoxicity

PP68

Rapid Green Synthesis of Bismuth Molybdate Nanoparticles for Wastewater Remediation

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ABSTRACT

Concerns about the removal of various organic poisonous are growing as a result of the overpopulation and the rapid growth of industry. The synthesis of a novel green photocatalyst with a high electron-hole separation and tremendous solar light harvesting capability is one of the most significant challenges in photocatalysis research. Herein, Bismuth molybdate nanoparticles were fabricated via green hydrolysis method in replacement of hazardous chemicals. The nanoparticles were synthesized using neem extract and were further tested for photo-degradation of organic pollutants under UV and visible light spectrum range. The photocatalytic results were compared with the pristine bismuth molybdate (BMO) nanoparticles which were synthesized without neem extract. The Green BMO showcased higher photoactivity in degradation of organic pollutants as compared to pristine BMO under visible light spectrum.

PP69

Preparation and Characterization of Poly (methyl Methacrylate-co-butyl acrylate-co-Acrylic acid)/bentonite Nanocomposites by Mini-emulsion Polymerization for Functional Coatings

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ABSTRACT

High solid polymeric coatings have become the center of attraction as they offer variety of benefits as compared to solvent-based coatings like increased durability, improved adhesion, less environmental impact, lower cost, faster drying time, etc. In this study, we are incorporating bentonite clay (0.25 - 1.0 wt%) in high-solid acrylic emulsions to enhance thermal properties, mechanical, anti- corrosive, and anti-microbial properties. High solid (~59%), bentonite-acrylic latex has been prepared, by using an acrylic copolymer of poly (methyl methacrylate-co-butyl acrylate-co-Acrylic acid) [P(BA-co-MMA-co-AA)]. All the stable latexes are successfully prepared by the mini emulsion technique. Here, sodium lauryl sulfate as surfactant and 1-butanol as co-surfactant, potassium peroxyorthosulphate as an initiator in the polymerization process. The influence of bentonite clay in the high solid emulsion was analyzed by DLS for particle size, viscosity, and film formation. The obtained free-standing films were characterized by FTIR, UV-visible spectrometer, DSC, TGA, UTM, anticorrosion and anti-microbial studies respectively. All latexes are stable for more than one month, composite films showed good thermal and mechanical properties.

Keywords: High solid acrylic emulsion, coating, entonite clay, anti-corrosive and anti-microbial.

Recent Advancement of Radiopharmaceuticals to be used in Nuclear Medicine

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ABSTRACT

Nuclear medicine is a branch of medical sciences that uses radioactive materials having the chemical composition in diagnosing and treating certain illness. These procedures use radioactive materials called radiopharmaceuticals. The radiopharmaceuticals used for diagnosis purpose are-(a)Abscess and infection-Gallium Citrate(Ga67) , Indium (In111) oxyquinoline (b) Billary tract blockage, Technetium Tc99m Disofonin, Technetium Tc99m Idofenin , Technetium Tc99m mebrofenin, C- Blood volumes studies – radio iodinated Albumin, Sodium chromate Cr57 and many more.

There are certain conditions required for an ideal radiopharmaceutical which include short half-life isotope, energy range, pure gamma emitter or beta emitters, target to non-target ratio, localization only in tissue desired, easy preparation and last economy price. Due to its potential use in a number of areas, such as radiation dosimetry, medical imaging, and environmental monitoring, these materials have attracted a lot of attention.

In this paper we have discussed how different radiopharmaceuticals and their collides are prepared using different techniques.

Keywords: Radiopharmaceutical, beta and gamma emitter.

PP71

Radiation-induced Skin Reactions: Mechanism and Treatment

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ABSTRACT

Radiotherapy (RT) is a major treatment for malignant tumors. The latest data show that >70% of patients with malignant tumors need RT at different periods. Skin changes can be experienced by up to 95% of patients who underwent RT. Inflammation and oxidative stress (OS) have been shown to be generally associated with radiation-induced skin reactions (RISRs). Inflammatory response and OS interact and promote each other during RISRs. Severe skin reactions often have a great impact on the progress of RT. The treatment of RISRs is particularly critical because advanced RT technology can also lead to skin reactions. RISRs are classified into acute and chronic reactions. The treatment methods for acute RISRs include steroid treatment, creams, ointments, and hydrocolloid dressings, depending on the reaction grading. Chronic RISRs include chronic ulcerations, telangiectasias, and fibrosis of the skin, and advanced treatments such as mesenchymal stem cells, hyperbaric oxygen therapy, superoxide dismutase, and low-intensity laser therapy can be considered. Here, we review and summarize the important mechanisms that cause RISRs as well as the standard and advanced treatments for RISRs.

PP72

Design and Development of Quinazolinone based Fluorescent Chemosensor for Selective Determination of Toxic Metal Ions in Environment Samples

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ABSTRACT

Design and development of optical probe chemosensor for selective determination of toxic metal ions in environment samples. Detection and quantization of selective metal ions such as Na(I), K(I), CA(II), Mg(II), Cr(III), Mn(II), Fe(III), Co(II), Ni(II), Cu(II), Zn(II), Cd(II), Hg(II) and Al(III) is done with chemosensor. The optical probe can selectively detect cations and anions through colorimetric or fluorometric responses. Various analytical methods including 1H NMR, 13C NMR, FTIR, TGA, SEM and ICP-OES are applied for structural characterization that further support the suggested chelation to ions through ligand. The metal binding character will be determined through UV-vis and fluorescence spectroscopy. Quantitative analyses of metal ions require advanced equipment like AAS, ICP-OES, SEM, XRD. A huge amount capital budget is required and tedious sample preparation. The same can be done with the development of new chemosensor with less cost. Therefore, this chemosensor can be considered promising chemosensor for detection of various ions in the environment samples.

PP73

Synthesis of Dual Responsive Monomer for Developing Soy Protein Hydrogels

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ABSTRACT

This work reports synthesis of novel monomer to prepare HLB-modified hydrogels by curing epoxy monomer with hydroxy group. The monomers will be studied for their amphiphilic behavior, swelling considerably both in organic solvents and in aqueous media. PEG chain shows hydrophilicity which can be modified by protecting the free hydroxyl group to alter hydrophilic lipophilic balance. The presence of pyridine moiety gives pH sensitivity, in acidic medium pyridine exists as pyridinium ion. The synthesized monomers will be used for developing soy protein hydrogels.

Keywords: Dual responsive Monomer, hydrogel, pyridine

Transition Metal Dichalcogenide-based Biosensor for the Detection of Tuberculosis at Early Stages

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ABSTRACT

Modern transducer technology has opened new possibilities for the construction of more precise and sensitive biosensors thanks to recent advancements in artificial intelligence (AI) and nanoscience. Transition metal dichalcogenides are garnering interest due to their widespread characteristics of changeable bandgaps, layered structure, cost-effectiveness, and ease of accessibility for a broad spectrum of bio-analytes. Among them MAX phases are garnering interest due to their nanolayered, hexagonal structure ($P6_3/mmc$ symmetry), they act as a transition between ceramics and metallics, being soft at room temperature and plastic at higher temperature ranges. It can be represented as $M_{n+1}AX_n$ (M= transition metal, A group III/IV elements, X= carbide/nitride/carbonitride). To date ~160 MAX phases are known out of which Ti_3AlC_2 and Ti_2AlC are most studied owing to their excellent thermal expansion coefficient, conductivity, and hydrophilicity which made them better options for biosensing. Herein, we demonstrated the extraordinary capability of Ti_3AlC_2 for the detection of the world's deadliest disease tuberculosis caused by Mycobacterium tuberculosis.

Keywords: chalcogenides, biosensors, 20D materials, *M. tuberculosis*

An Update on the use of Organic Materials as Detectors in Radiation Detection

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ABSTRACT

Radiation detectors have broad applications in various fields such as nuclear physics, astrophysics, medical diagnosis research etc. Modern detectors system consists of two components, the detector which may be gas filled detector, semiconductor, and scintillator detector and a closely associate instrumentation that provide the actual measured signal. Performance of radiation detection is based on energy resolution, spatial resolution, detection efficiency.

Scintillation detectors are more robust for field deployment and are often chosen over semiconductors due to substantially favorable cost. Though both inorganic and organic materials can serve as radiation detectors. However, more and more research is happening in the field of organic Scintillators such as Halide Perovskites for X-ray Detection because of low cost, custom made, etc. Due to their exceptional inherent electrical and optical properties, ease of processing using simple solutions, and economic feasibility, halide perovskites have emerged as model materials for X-ray detection and imaging, such as large absorption coefficient, high Photoluminescence quantum yield, tunable bandgap, and long carrier lifetime.

Keeping in view of the raising needs in the field of medical radiation, this review has been under study. The scope of the investigation could result into synthesis of more reliable, low cost, and high quantum detection organic materials.

Study of Chemical Composition of Different Radionuclides used in Preparing Radio Pharmaceuticals

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ABSTRACT

With the growth of number of cancer cases, use of radiopharmaceuticals has increased many folds in the past many years. Radiopharmaceuticals effectiveness and specificity are primarily influenced by their chemical make-up and the kind of chemical bond they form with the molecules.

Radioisotope like rhodium-188 has demonstrated tremendous promise for use in radiopharmaceutical because of its favorable nuclear decay characteristics and capacity to form long-lasting chemical bonds with target molecules.

Another radioisotope 99mTc, which is present in 28 radiopharmaceuticals that have received FDA approval. There are currently two agents available; one is 99mTc-DTPA with an unknown structure, and the other is [99mTcO(MAG3)]. It is common practice to use 99mTc complexes with phosphonate ligands as diagnostic tools for the identification and follow-up of metastatic illness in infections of the bone and bone infarction. Another radioisotope ^{64}Cu is used as a companion diagnostic agent to select and plan for therapeutic applications using the β^- emitting isotope.

In this paper, chemical bonding in all various radioisotopes is discussed and their role in the formation of chemical bonds and its use in radiopharmaceutical applications is the main study of this paper, with recent developments and suggests future research paths.

Keywords: Radiopharmaceuticals, radioisotopes, chemical bonds

Removal of Ni^{+2} from Aqueous solution using Carbon Nanosheets (N-CNS)

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ABSTRACT

Nickel (Ni^{+2}) is a toxic heavy metal releasedwith different industrial effluents, its presence in water causes serious problem to environment as well as to human health. Adsorption is one of the most studied technologies, due to its higher removal efficiency and easy operational process. However, finding a suitable, effective and environmentally convenient adsorbent is still under research. For this purpose, the present study aims to synthesise nitrogen doped carbon nanosheets(N-CNS) using melamine, glycerol and sulphuric acid via a hydrothermal process. Synthesised N-CNS was amorphous in nature with porous and layered morphology and 1-4 nm height profile. N-CNS was applied for the adsorption of $Ni^{+2}$from aqueous solution. A maximum 83.09 % adsorption of $Ni^{+2}$was observed using initial 20 mg/L concentrationof Ni^{+2}. The optimum conditions found for the maximum adsorption of $Ni^{+2}$by N-CNS were: adsorbent dose 0.5 g/L, pH 6,Ni^{+2}concentration 20 mg/L. A slight increase in adsorption percentage was reported with increase in temperature from 30 to 50 ˚C. Maximum adsorption capacity (Q_0) of N-CNS was found to be 43.54 mg/g. The adsorption data was also analysed by the application of two adsorption isotherm models and the adsorption of $Ni^{+2}$was followed best by Freundlich isotherm with value of R^2 to be 0.824.

Profiling of Nitrosamine Impurities in Active Pharmaceutical Ingredient

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ABSTRACT

The term "active pharmaceutical ingredient" refers to a substance or a compound that is meant to be used in the production of a pharmaceutical product as a therapeutically active substance. (API). Development of APIs involve use of variety of reactive elements such as starting materials, catalysts, chemicals, and intermediates. It has been observed that pharmaceutical ingredient is associated with trace amounts of reactive impurities, some of them have been categorized as genotoxic impurities (GTIs) based on their composition and reactivity. One such example is nitrosamine impurities. FDA accentuated that the source of nitrosamines can be related to the drug's manufacturing process or the chemical structure of drug as well as the storing/packaging conditions. It is to be noted that eight types of nitrosamine impurities (NDMA, NDEA, NEIPA, NDIPA, NDPA, NMPA, NDBA, and NMBA) have been identified. These impurities are separated from each other as well as from the metformin by reverse phase chromatography and are detected by a high-resolution and high-mass accuracy (HRAM) mass spectrometer. The present work involves the synthesis and characterization of the nitrosamine impurities.

Keywords: Impurities, Active Pharmaceutical Ingredient, Nitrosamine

Ocimum Sanctum Based Hybrid Ferrite Nanocomposite: An Advance and Sustainable Material for Water Cleansing

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ABSTRACT

The purpose of the study was to fabricate sustainable and cost-effective material for the thorough cleansing of polluted water. In this context, an economical, Ocimum sanctum plant-based nanocomposite material, CoFe2O4/OS, was prepared via co-precipitation technique. A thorough analysis for its characterization was conducted using several spectroscopic and microscopic techniques. The characterization results showed that the magnetic nanocomposite exhibited substantial functional groups of Ocimum sanctum powder and magnetic ferrite part. The adsorption investigation of nanocomposite for removal of two cationic dyes was carried out with varying parameters, such as pH, contact time, temperature, concentration, and composite dosage. The facile preparation, economical cost, significant magnetic character, will surely construct the water treatment system more competent with the use of CoFe2O4/OS.

Keywords: Adsorption, Cobalt Ferrite, Magnetic nanocomposite, Wastewater treatment

Quality Control Methods to Check Phthalates Toxicity in Textile Products

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ABSTRACT

Based on quality testing, this review seeks to comprehend the toxicity of phthalates in textile products. Quality control is defined as the guidelines that are designed to meet the product's specific required standard. In textile products such as garments, the quality control method that is opted in phthalates is CPSC-CH-C1001-09.4. This method is divided into three sections: sample preparation, extraction, and analysis. This method is used to determine the concentration of phthalates in consumer products like coating, children's products and polymers. The limit of detection is 50ppm and the failed limit is 1000ppm.

GC-MS is recommended for analysis because it helps to separate, detect and identify the class of target compounds based on their physical and chemical properties.

Phthalates are one of the performance parameters that have recently raised concerns about both human health and the environment. Phthalates are a type of plasticizer that increases the space between polymer chains, increasing flexibility and durability. It is a man-made chemical that primarily causes endocrine disorders, decreased fertility, cancer, and diabetes. Phthalates are used in textile products such as printed inks and active wear to enhance the properties. The increase of phthalates in the environment has caused an increase infertility-related medical problems in recent years. It has a wide range of industrial applications and is easily released from plastics into water.

Keywords: Phthalates, health risks, GC-MS, extraction technique, phthalates exposure

ABOUT AIAS

Amity Institute of Applied Sciences (AIAS) was established under the aegis of Amity University, Uttar Pradesh with a vision to be a Center of Excellence for Physical, Chemical, Mathematical and Statistical Sciences. The institute's highly qualified faculty includes more than 98% doctorates. AIAS offers UG, PG and doctoral programs in Physics, Chemistry, Mathematics, Statistics and Medical Physics. It has research collaborations with the labs of Govt. of India as well as international universities and research institutes. The highly research oriented faculty regularly publishes papers in journals of high repute. AIAS faculty has filed a number of patents and has got sanctioned projects from premier funding agencies. Conferences, seminars and workshops are organised frequently.

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