CONFERENCE PROCEEDINGS

INTERNATIONAL CONFERENCE ON
FRONTIER AREAS IN CHEMICAL TECHNOLOGIES - 2024

22nd & 23rd March 2024

Editors
Dr. M. Sundrarajan
Dr. T. Stalin
Dr. G. Gopu

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KARAIKUDI – 630 003, Tamil Nadu, India

International Conference on
FRONTIER AREAS IN CHEMICAL TECHNOLOGIES - 2024
Conference Proceedings

Editors
Dr. M. SUNDRARAJAN
Dr. T. STALIN
Dr. G. GOPU

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PREFACE

Chemical technologies encompass challenging and fascinating fields; including electrochemistry, textile chemistry, nanochemistry, green chemistry, materials chemistry, computational chemistry, and more. These technologies find applications in nearly every field of science and technology. Researchers, educators, and developers working in academic institutions and industry are focusing on the latest advancements in research and development related to chemical and electrochemical sciences and technologies. The present conference on **Frontier Areas in Chemical Technologies (FACTs-2024)** is the iconic annual International Conference organized by the Department of Industrial Chemistry to focus on the update of recent advancements in different areas of chemical science and technologies. The aim of this international conference is to provide a forum to all the chemists, physicists, biologists and material scientists, technologists and researchers to discuss their recent findings and information and to promote cooperation both nationally and internationally. The invited talks and papers focus mainly on various advanced aspects of Chemical Technologies such as¯ Electrochemical Technologies, Nanoscience and Technology, Sensor Technologies, Supramolecular and Photochemical Technologies, Green Chemical Technologies and other alliedtechnologies.

It is indeed a matter of great pleasure and satisfaction to the Editors to present this volume containing collection of abstracts to be presented in the International Conference on FACTs- 2024 at Alagappa University, Karaikudi during 22nd and 23rd March-2024. There are about 12 Invited Talks, 45 Oral Presentations and 85 Poster Presentations. In addition, the programme includes open forum discussions. About 250 delegates from various Research Institutes, Universities, Colleges and Industries in India including four Invited Speakers from overseas participate in the conference.

The editors are thankful to **Prof. G. Ravi**, Vice-Chancellor, Alagappa University, Karaikudi for supporting all the activities of this International Conference and advising in strengthening the research culture among the young researchers. Our sincere thanks are to **Dr. A. Senthilrajan,** Registrar, all the **MembersofSyndicate**and Authorities of Alagappa Universityfor their constant support and encouragement. Sincere thanks are due to the Organizing Committee Members of the conference, Faculty Members, Research Scholars and Students of the Departments of Industrial Chemistry. We also thank all the authors for submitting their abstracts in time.

We wish all the delegates to have pleasant stay in Karaikudi and stimulating discussions during the International Conference on FACTs-2024.

Editors
Dr. M. Sundrarajan
Dr. T. Stalin
Dr. G. Gopu

ALAGAPPA UNIVERSITY
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Prof. G. Ravi, Ph.D., D.Sc.,
Vice-Chancellor

MESSAGE

I am very happy to note that the Department of Industrial Chemistry is organizing an "International Conference on "Frontier Areas in Chemical Technologies - 2024 (FACTs-2024)" and also celebrating World Water Day on 22nd and 23rd March 2024.

The theme of the conference is to provide a platform for the young researchers to expound and bring forth the latest advances in the field of Chemical Technologies. Chemical technology is a branch of chemistry concerned with creating new chemical products. Chemistry is the scientific study of the transformation of substances. It includes chemical reactions and other transformations like distillation or grinding. Chemical Engineering Science, on the other hand, deals with the physical, mechanical, physicochemical, and chemical aspects of all industrial processes that involve the transformation of substances.

Chemical technologies are a fascinating and challenging branch of Chemistry with diverse applications in various fields of science and technology. Therefore, it is highly appropriate that the Department of Industrial Chemistry is organizing an international conference with invited lectures from renowned personalities and paper presentations by academicians, scientists, scholars, and industrialists.

I am sure that all the delegates would be greatly benefited by the deliberations and this Conference will undoubtedly emerge with many innovative ideas for the young researchers in the frontier areas.

I wish the conference a grand success.

VICE-CHANCELLOR

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Padma Bhushan
Vallal Dr. RM. Alagappa Chettiar

Dr. **A. SENTHILRAJAN**
Registrar

Date: 18.03.2024

MESSAGE

The Department of Industrial Chemistry is organizing an International Conference on "Frontier Areas in Chemical Technologies-2024 (FACTs-2024)" and celebrating World Water Day on March 22–23, 2024.

The main objective of the conference is to provide a platform for emerging researchers to discuss and present the latest developments in chemical technologies. Chemical technology is a field of chemistry that focuses on the development of innovative chemical products. This sector also includes the scientific study of substance transformation, known as chemistry, which involves chemical reactions and other transformations. Chemical Engineering science deals with the physical, mechanical, physicochemical, and chemical aspects of all industrial processes involving the transformation of substances. Chemical technologies are a fascinating and challenging branch of chemistry with diverse applications in various fields of science and technology. Therefore, it is highly appropriate that the Department of Industrial Chemistry has organized an international conference.

The conference will feature invited lectures from renowned personalities, as well as paper presentations by academicians, scientists, scholars, and industrialists.

I wish the Conference an immense success.

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KARAIKUDI - 630003, Tamil Nadu, India

Dr. M. SUNDRARAJAN, Associate Professor and Head i/c, Convener, FACTs – 2024

WELCOME TO THE DELEGATES

On behalf of the Staff and Students of the Department of Industrial Chemistry, Alagappa University, Karaikudi, I am pleased to extend a hearty welcome to all the delegates of the International Conference on Frontier Areas in Chemical Technologies (FACTs – 2024) during 22 – 23 March 2024.

Though the conference announcement was at short notice, there was an overwhelming response. About 165 technical papers and 12 Invited Lectures have been received during this short notice of time. These cover a wide range of topics and are programmed to be deliberated in 4 technical sessions.

I am delighted to the response received from Academicians, Scientists from R & D Institutions and Chemists from Industries. The Conference would also provide a common platform to share their ideas or achievements of research into industrial applications to reach the common man and also help to establish a strong academic – research – industrial relationship. I hope that, the Conference will provide the unique opportunity for participants to interact and share the knowledge and experience.

I wish the delegates for an enjoyable and memorable stay at Karaikudi.

Dr. M. Sundrarajan

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INVITED TALKS (IT)

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INVITED TALKS
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IT-01

WATER FOR PEOPLE, WATER FOR LIFE - ELECTROCHEMISTRY IN ACTION

S. Vasudevan

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Abstract

Water the generous gift of nature is sure to become scarce unless the ever-growing population is enlightened enough in handling the increasing stress and to avoid the crisis due to the expanding demand on this precious commodity. Management of water and its resources by conservation and its judicious use help to preserve the available water. Even then, whether it is from surface or underground sources, it has become impossible to obtain good quality water for human consumption. Thus, the dwindling quantity and lessening quality of water require effective steps to be taken urgently for the sustenance of the living being of today and tomorrow.

The extent of water contamination is so much and so varied that organic, inorganic and biological impurities are present in the water due to natural as well as induced reasons. The responsibility fell on the scientists and engineers to provide appropriate technologies not only to prevent the pollution at the source itself but also to treat at the user end.

The conventional processes for pollution abatement are either physicochemical or biological. The physicochemical methods aim at shifting the pollutants (land fill), concentrate the pollutant (adsorption), transfer the pollutant to another medium (air stripping) or cause secondary pollution (chemical precipitation leading to sludge). Biological techniques require narrow range of operating conditions. Electrochemistry provides technologies that have definite advantages than the above conventional methods.

Water quality up-gradation by electrochemical technique presents various alternatives, such as anodic, cathodic, direct and indirect methods to treat any type of contaminants in water and waste water. These methods, at the point of entry of pollutants into the environment, help not only to remove the contaminant but also to recover and recycle useful chemicals. The electro-remediation of contaminated soil is, now, a proven and viable technology to prevent the pollution of water at the point of contamination itself.

In this context, my talk will be the environmental applications of electrochemistry and some of the important and recent developments in the electrochemical methods of water treatment are reviewed. Electrochemical processes for decontamination of drinking water developed by CSIR-CECRI are also briefly described.

IT-02

CHARGE TRANSFER IN NANO-ARCHITECTONIC HETEROJUNCTIONS: IMPORTANCE IN ARTIFICIAL PHOTOSYNTHESIS

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TC
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Abstract

This talk focuses on the importance of heterojunction photocatalysts and their charge transfer behavior. Some basic concepts that must be taken into account during its use in energy and environmental catalysis will be covered, which touch on the following topics:

- Water splitting with semiconductor-photocatalysts
- Problems associated with single semiconductor photocatalysts and howheterojunctions can overcome these problems.
- Design of heterojunctions and their characterization using various techniques to understand the behavior of charge transfer.

In addition, recent work on energy and environmental catalysis through heterojunctions that we developed in the materials science group will be briefly discussed.

Keywords: Heterojunctions, Photocatalyst, charge-transfer, Energy and Environment

IT-03

SYNTHESIS OF BIOACTIVE COMPOUNDS UTILIZING UMPOLUNG REACTION OF A-IMINO ESTER ANALOGUES

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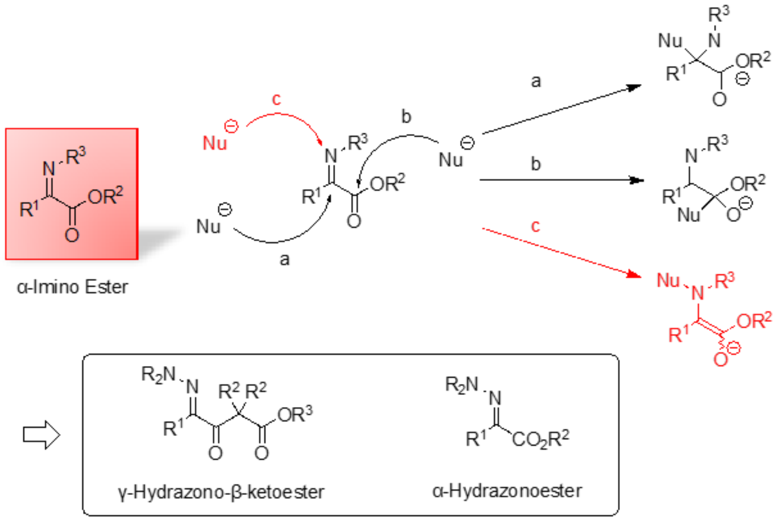
Abstract

α-Imino ester has an ester moiety located next to the imino carbon. Since this decreases the LUMO energy and increases the electrophilicity of the imino carbon, these are known as reactive imines and are often used as precursors to α-amino acid derivatives. The nucleophilic addition usually occurs at the imino carbon or the ester moiety (path a and b), leading to the preparation of tertiary or quaternary α-amino acids and amino ketones. On the other hand, the imino nitrogen rarely behaves as the electrophilic center. This reaction is impossible unless the polarity of the imine is reversed, and it's called an umpolung reaction (*N*-alkylation). This type of reaction also generates an enolate which reacts with various electrophiles to give a new C-C bond formation (path c).

Although an umpolung reaction for α-imino ester was first reported by Kagan in 1971 during the addition of Grignard reagents to α-imino esters, no vigorous research has been investigated due to their difficulties and limitations. We have developed umpolung reactions of α-imino esters and various tandem C-C bond formation reactions using the metal enolate produced by *N*-alkylation.[1] Herein we disclose new types of tandem reactions utilizing umpolung reactions of α-imino ester analogues such as γ-hydrazono-β-ketoester[2] and α-hydrazonoester[3] for syntheses of bioactive compounds.

Keywords: α-Imino Esters; Umpolung Reaction; *N*-Alkylation; Tandem Reaction; Hydride

Reduction; Amidation; Bioactive Compounds



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IT-04

CONJUGATED POLYMER FRAMEWORK OR NETWORK AND THEIR APPLICATIONS

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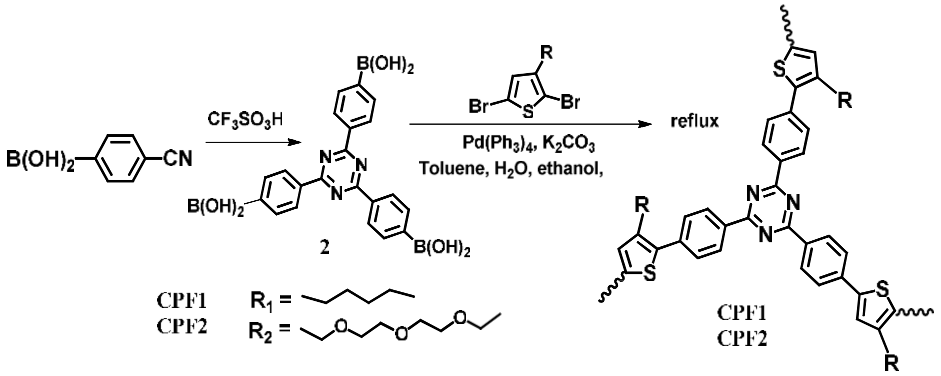
Abstract

Conjugated polymer framework (CPF) or network (CPN) have recently attained tremendous research attention due to their multifaceted applications including energy storage [1], catalysis [2] and separation [3] that originates from their unique combinations of properties like extended π conjugation, microporosity and high surface area. These framework materials, without sidechains or functional groups on their back bone, are generally insoluble in common organic solvents. Whereas, CPF with sidechain are solution processable for electronic device applications. Herein, we have recently developed a series of triazine based conjugated polymer framework (CPF) by conjugating different moieties like thiophene, carbazole, fluorene unit with triazine ring through a phenyl ring linker. The effect of side chain polarity on self-assembly, photophysical, electrochemical, band gap and electronic property of these CPF were also systematically studied. When these CPFs were reacted with Lewis acids and bases, significant optical switching and conductivity changes were observed indicating efficient nonoxidative doping/dedoping. Both CPF exhibit remarkable stability after several switching cycles from neutral to doped states and vice versa. These materials show a wide range of potential applications ranging from catalysis, electrocatalysis, electrochromism, and electroluminescence. Synthesis scheme of such thiophene and triazine based CPF is shown in Figure 1.

Keywords: Conjugated polymer, Conjugated polymer framework, Electrochromism, Electrocatalysis.



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IT-05

CATALYTIC AMIDATION A GREENER AND ECONOMICAL ALTERNATIVE

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Abstract

Amide derivatives are very important molecules in the pharmaceutical industry, notably up to 65% of drug molecules contain amide units in their structure. In addition, amides are widely used in agrochemical production, pesticides, and polymers materials such as synthetic silks, nylon, etc. Notably, most of the chemical and pharmaceutical industries still use various coupling or activating agents for amide synthesis resulting in the generation of a stoichiometric amount of waste that is toxic to the environment and has a poor atom economy. Therefore, American Chemical Society Green Chemistry Institute Pharmaceutical Roundtable (ACS GCIPR) has identified an Amide bond forming reaction by avoiding poor atom economy reagents as the high priority area of research for the pharmaceutical industry. We are trying to address this challenge by developing new catalytic, economical, and environment-friendly protocols for amide synthesis. Based on our continuous interest in developing new methods for catalytic amidation so far, we have explored phosphorus[1] and boron-based catalysts,[2-3] metal catalysts.[4-5] Currently, catalytic amide synthesis is one of our main focus areas of research.

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IT-06

SEAWEED BIOREFINERY: BLUE CARBON TO BIOFUELS AND FINE CHEMICALS

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Abstract

Macroalgae have been recognized as a source of functional ingredients with positive health effects, due to the presence of highly beneficial, immune-boosting functional polysaccharides. Recently, macroalgae have also been recognized as a potential feedstock for producing biofuels and bio-based chemicals. Macroalgae are classified based on their pigmentation into three types – green algae, red algae, and brown algae. The carbohydrate content of macroalgae is over 50%, which makes them a suitable substrate for microbial fermentation and bio-conversion.

For the first time, dark fermentation of the green macroalgae Ulva sp. for biohydrogen production was explored. A combined mild acid–thermal pretreatment resulted in a 42% reducing sugar recovery. Anaerobic fermentation with Clostridium butyricum resulted in a cumulative hydrogen production, yield, and productivity of 2340 mL/L, 1.53 mol H_2/mole RS, and 208.3 mL/L/h, respectively. Continuous fermentation increased the productivity to 782.45 mL/L/h, superior in the renewable feedstock category. Furthermore, green, red, and brown macroalgae for the microbial production of lactic acid. Lactic acid is one of the few commodity chemicals for which bio-based products are predominant. *Ulva* sp., *Gracilaria* sp., and *Sargassum cristaefolium* were evaluated as a feedstock for LA fermentation. Mild acid-thermal hydrolysis (sulfuric acid concentrations <5%) resulted in superior reducing sugar recovery. Consistent high lactic acid yields of over 0.8 g LA per g sugars were obtained. Effective

fermentation of a fucose-rich macroalgal hydrolysate by lactobacilli with high lactic acid yields (0.81 g/g) was reported for the first time. *Lactobacillus plantarum* and *Lactobacillus rhamnosus* could efficaciously ferment the sugars derived from all the macroalgae.

We have shown that macroalgae can be considered a suitable substrate for biofuel and bio-based chemical production. Pelagic macroalgae can be effectively valorized in this manner, attaining value-added products and waste valorization simultaneously.

IT-07

DIVERSITY AND NEW DIRECTIONS OF NEW AGE NANOSTRUCTURED MATERIALS

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Abstract

Nanostructured materials are of interest because they can bridge the gap between the bulk and molecular levels and leads to entirely new avenues for applications, especially in electronics, optoelectronics and biology. When a solid exhibit a distinct variation of optical and electronic properties with a variation of particle size <100 nm, it can be called a nanostructure, and is categorized as two dimensional, e.g., thin-films or quantum wells, one dimensional, e.g., quantum wires, or zero dimensional or dots. During the last two decades, a great deal of attention has been focused on the optoelectronic properties of nanostructured semiconductors or quantum dots (Q dots) as many fundamental properties are size dependent in the nanometre range. A Qdot is zero dimensional relative to the bulk, and the limited number of electrons results in discrete quantized energies in the density of states (DOS) for non-aggregated zero dimensional structures. Sometimes, the presence of one electronic charge in the Qdots repels the addition of another charge and leads to a staircase-like I-V curve and DOS. The step size of the staircase is proportional to the reciprocal of the radius of the Qdots. The boundaries, as to when a material has the properties of bulk, Qdot or atoms, are dependent upon the composition and crystal structure of the compound or elemental solid. An enormous range of fundamental properties can be realized by changing the size at a constant composition and some of these are discusses. Qdots can be broadly categorized into either elemental or compound systems. Semiconductor-based nanostructured materials and their multimodal applications

based on optoelectronic and optical properties. Nanofibers have gained much interest for use in various biomedical applications over the past few decades due to their unique functional properties such as large surface area and high aspect ratio, which plays a vital role in cellular and molecular activities, and their structural similarity to native cellular microenvironment. Despite their numerous advantages, some of the biomedical applications require the use of nanofiber composites owing to their excellent structural and tunable functional properties compared to the monophasic nanofibers. Nanofiber composites are a relatively new, unique, and versatile class of nanomaterials. In future, it is believed that several strategies would evolve in the field of the fabrication of fibrous composite scaffolds for gene delivery, which will ultimately lead towards excellence, with better material properties and release profiles, and improved transfection efficiency.

IT-08

SOLID-STATE PHOTOCHEMISTRY OF *CIS*-CINNAMIC ACIDS: A COMPETITION BETWEEN [2 + 2] ADDITION AND *CIS-TRANS* ISOMERIZATION

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Abstract

The photochemical reactions and X-ray structural studies of *cis*-cinnamic acids in the solid-state, are carried out to understand the photochemical behavior of *cis*-isomers by exploiting topochemical postulates. Extensive research on the photochemistry of *trans*-cinnamic acids was well explored by Schmidt and co-workers.[1-6] Due to the limited availability of literature on *cis*-cinnamic acids,[7] the photochemistry of excited *cis*-cinnamic acids can be understood from the photochemistry of the corresponding *trans*-cinnamic acids but not from *cis*-cinnamic acids alone.[8] Existence of dual reactive centers and its photoreactivity of *cis*-olefinic crystals are thoroughly investigated.[8] Similar to *trans*-cinnamic acids, *cis*-cinnamic acids can also undergo direct photodimerization when the intermolecular distance of double bonds is less than 4.2 Å. The photochemistry of selective *cis*-cinnamic acids can dimerize via a diradical intermediate in the crystalline state when the intermolecular distance is less than 4.2 Å. In the excited state of *cis*-isomers, C–C bond formation with an adjacent molecule competes with geometric isomerization. In addition, the mechanistic interpretation of *cis*-olefins provides the much-needed foundation for future studies since the study of *cis*-isomers was overlooked in favour of the t*rans* isomer.

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IT-09

NATURE-INSPIRED MATERIALS FOR EXCITING APPLICATIONS

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Abstract

Bioinspired materials derived from natural sources such as plant and animal parts have the benefit of inheriting some of the properties of the raw materials, like macro- and micro-pore structure, optimal composition, similar morphology, etc., along with the advantages of unlimited worldwide availability at a very low raw material cost. Here, the demonstration of processes like self-assembly in lab conditions will be discussed, along with how these self-assemblies are useful in various bio- and engineering applications. Understanding the mechanism of natural processes will lead to the development of various products that will be a solution to the lifeline of the earth. In this aspect, some of the recent results obtained with self-assembled synthetic and natural nanomaterials will be discussed, along with their potential future applications.

IT-10

TURN-ON FLUORESCENT SENSOR FOR OXALIC ACID BASED ON DINUCLEAR ZINC COMPLEX

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Abstract

Oxalic acid (OA) is the simplest dicarboxylic acid occurring in various type of plants, vegetables and microorganism. Moreover, the concentration of oxalic acid in the urine is the primary measurement for renal stone diagnosis. These caused the urgent need to develop a novel strategy for accurate determination of OA content in food as well as wastewater. Therefore, rhodamin-6G based dinuclear zinc complex was designed as a fluorescent probe for the selective detection of oxalic acid (OA). Thus designed sensor exhibited rapid fluorescent “turn-on” response along with high selectivity towards OA over other dicarboxylic acids studied in H_2O: C_2H_5OH (8 : 2, v/v) at neutral pH. The absorption (531 nm) and fluorescent intensity (539 nm) of the receptor increased with increasing concentration of OA. In order to explore the efficiency of dinuclear zinc complex rather than the precursor towards the detection of OA, the absorption profiles of {[Rh-I-Zn^{2+}] + OA}, {[Rh-I] + OA} and {[Rh-I-OA] + Zn^{2+}} were examined. Among these, {[Rh-I-Zn^{2+}] + OA} exhibited very high absorption than other mixtures, indicating the efficiency of the binuclear zinc complex towards the detection of OA. Spectral characterization revealed that the amide from spirolactum ring open-form of the signaling unit (rhodamine) and the zinc complexes are the two binding sites for the selective coordination of OA. The reversibility of the sensor can be achieved by the treatment with sodium sulfide which regenerated the intermediate. The limit of detection (LOD) of [Rh-I-Zn^{2+}] towards OA was found to be 1.20 μM, which are comparable to most of the fluorescence.

IT-11

RESEARCH PROGRESS IN THE DEVELOPMENT OF DSSC

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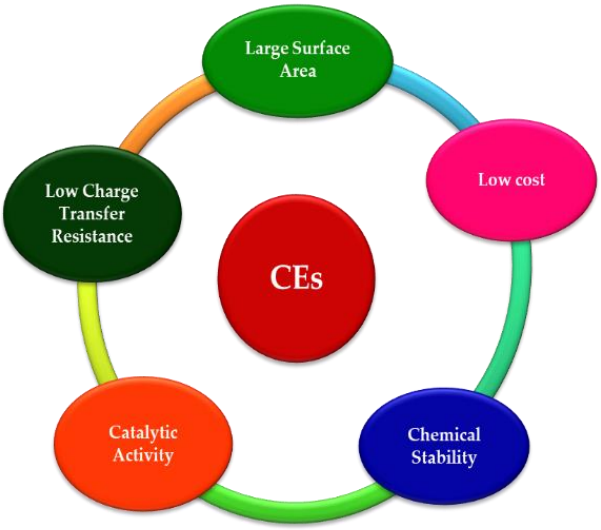
Abstract

A dye-sensitized solar cell (DSSC) has been considered as a cost-effective alternative to silicon-based solar cell and achieved a maximum power conversion efficiency (PCE) of 13%. In order to enhance its power conversion efficiency, one of the essential ways is to improve the fill factor by modifying the counter electrode. The high cost of DSSC is mainly due to the high loading of Pt that required to catalyze the tri-iodide reduction reaction. In order to reduce the cost of DSSC, efforts have been made to find out cheaper alternative CEs for DSSC. This lecture gives a concise overview of alternative CE materials such as Pt-free alloys, Graphene, Carbon nanofibers, conducting polymers, Chalcogenides and their nanohybrids.[1-5] Besides that the power conversion efficiency, cost and stability of theit device are compared. This talk end-up with the conclusion and future prospects.



Properties of Counter Electrode

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IT-12

REVOLUTIONIZING THE WORLD WITH INNOVATIVE AND ENVIRONMENTALLY BENIGN ENERGY CONVERSION DEVICES

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Abstract

Tackling environmental challenges today is more of an investment for the future than a mere expense. It's our duty in the modern era to safeguard the natural splendor and riches passed down by previous generations for those yet to come. The urgent need for new, sustainable energy solutions has been sparked by the global surge in energy demand and the dwindling supply of fossil fuels, focusing on converting waste into energy. Although sustainable fuels might offer higher energy densities compared to compressed hydrogen, the actual power efficiencies of the associated fuel cells are significantly lower than those found in traditional fuel cells. Direct urea fuel cells (DUFCs) and microfluidic ethylene glycol fuel cells (µDEGFCs) show promise as devices for converting energy sustainably; however, the lack of effective electrocatalysts for fuel oxidation and the oxygen reduction reaction remains a major hurdle to their widespread adoption. To overcome this, µDEGFCs and DUFCs were developed using 3D carbon aerogels (CAs) that contain bimetallic nanoparticles within carbon nanotubes (CNTs) and are structured with precisely patterned microfluidic channels. The innovative catalytic 3D nanostructures and direct electrode integration achieved maximal power densities and exceptional longevity, vastly surpassing the performance of previously reported catalysts. This lecture will explore viable strategies to overcome the current limitations of eco-friendly fuel cells and broaden their application in real-world scenarios.

IT-13

MOLECULAR ENGINEERING OF CUCURBITRUIL-BASED ALGINATE HYDROGELS

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Abstract

My team in UAEU designs and creates new biopolymer hydrogels utilizing a non-classical approach (non-covalent interactions). Inspired by biological systems, the new supramolecular architectures have inherent (dynamic) reversibility and responsiveness to chemical and thermal stimuli for applications in biology, agriculture, and the environment in the UAE and across the globe. This talk explains how several alginate hydrogels are engineered in our lab by grafting small molecules and macromolecules onto alginate solid platforms (biopolymers). Such a facile combination obviates the need for multiple steps in organic reaction, highlighting our research's merit. Our specific inspiration lies in utilizing the unique supramolecular recognition properties of cucurbituril (CB) macrocycles, such as their ultrahigh affinity and preferential binding towards the protonated forms of the guest molecules over the neutral forms. The talk will then specifically highlight how the CB hosting property was utilized to covalently link a supramolecular host-guest complex of viologen diamine (VG) and CB8 to the surface of alginate polysaccharides (ALG). The complexation in CB8 turns over the charge and decreases the size of VGALG hydrogel, enabling it to enter the blood cancer cells. This presentation also highlights using time-resolved solid optical measurements in our CB research.

keywords: Alginates; Cucurbiturils; Hydrogels; Biomaterials.

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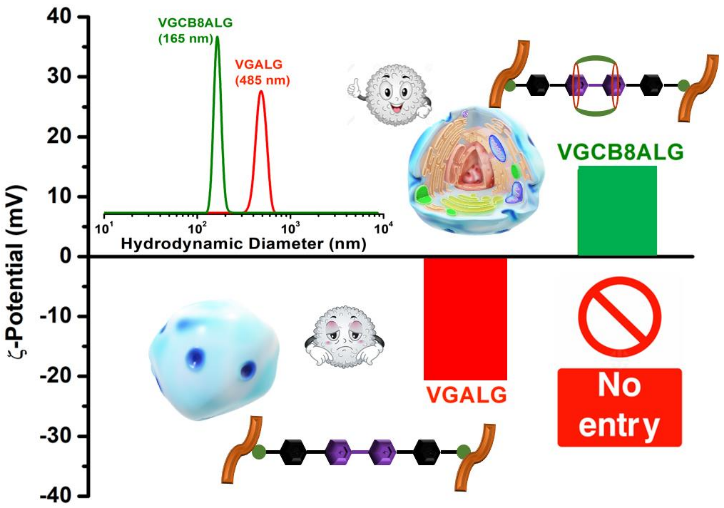

Figure. CB8 turns over the charge and decreases the size of VGALG hydrogel, enabling it to enter the blood cancer cells.

IT-14

SELECTIVE ELECTROCATALYTIC REDUCTION OF CO_2 TO FORMIC ACID AT LOW OVERPOTENTIAL IN WATER USING Mes-$IrPPh_2$ COMPLEX

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Abstract

As a solution to the current global energy and environmental crisis, electrochemical and photocatalytic conversions of carbon dioxide (CO_2) are being investigated as promising methods for converting CO2 into valuable carbon resources. Numerous studies have been conducted on the development of catalysts for CO2 electrochemical reduction (CO2ER), but their performance has yet to be deployed for large-scale applications due to their low durability and reusability. The most promising approach to molecular catalyst heterogenization on electrode surfaces involves reducing catalyst loadings, improving electron transfer efficiency, and preventing any deactivation of catalysts caused by steric confinement.[1] In our laboratory, molecular iridium (Ir) complexes with PNNP-type tetradentate ligands have shown superior performance in converting CO_2 to formic acid (HCOOH) under photoirradiation with high reactivity and selectivity with sacrificial electron donor 1,3-dimethyl- 2-phenyl-2,3-dihydro-1H-benzo[d]imidazole (BIH).[2]

By heterogenizing the catalyst on the surface of the carbon electrode, the Ir complexes were successfully utilized to catalyze CO2ER in an aqueous solution. Under optimized conditions, CO2ER was efficiently facilitated at a very low overpotential (ca. 100 mV) to furnish mainly HCOOH with a current density of 8.4 mA cm^{-2} at −0.28 V vs RHE. Employing

this cathode catalyst, both high product selectivity (94%) for HCOOH and Faradaic efficiency (> 90%) were achieved in an aqueous solution, where CO_2ER competes in selectivity with H2 evolution. In my talk, I’ll introduce tetradentate PNNP type metal complexes for the electrocatalytic CO2 reduction and their reaction mechanisms.

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ORAL PRESENTATION

(OP)

OP-01

SEQUENTIAL USE OF DIELS-ALDER, REDUCTION, FLUOROCYCLIZATION REACTION FOR THE ORGANOCATALYTIC ASYMMETRIC CONSTRUCTION OF OCTAHYDROFURANOINDOLE CORE FOUND IN ASPIDOSPERMA ALKALOIDS

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Abstract

The advent of trienamine catalysis has revolutionized the field of organic synthesis by offering a gentle yet efficient method for crafting complex carbocyclic frameworks in a single step via distant [4+2]-cycloaddition reactions. While the application of dienals or dienones in trienamine catalysis is well-documented, the use of heteroexocyclic dienals remains relatively unexplored. Motivated by the biological importance and unique reactivity of oxindole olefins, our research explores their feasibility in trienamine catalysis for our target dienal. In this work, we report the enantioselective creation of new fluoro-octahydrofuranoindole spirooxindoles, characterized by five consecutive stereocenters, through an organocatalytic sequence combining Diels-Alder reaction, reduction, and fluoroetherification. We successfully extended this innovative method to synthesize a varied collection of compounds, achieving up to 20 examples that mimic the backbone of certain natural substances. These compounds were synthesized with moderate to high efficiency and showcased exceptional diastereo- and enantioselectivity, achieving as high as 77% total yield, 99% enantiomeric excess (ee), and a diastereomeric ratio (dr) of 10:1.

Keywords: Aspidosperma alkaloid, Diels Alder, Asymmetric synthesis, organocatalysis, fluoroetherification.

OP-02

HUMAN CONSUMPTION RISK AND METAL BIOACCUMULATION IN THE TISSUES AND SHELLS OF EDIBLE BIVALVES *Callista erycina* AND *Pinctada fucata* ALONG THONDI COAST, PALK BAY, INDIA

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Abstract

Using inductively coupled plasma mass spectrometry (ICP-MS), the bioaccumulation of metals in shells and tissues of the 2 different edible bivalves (*Callista erycina* and *Pinctada fucata*) was investigated and potential ecological and human health risk assessment were also studied. Totally 17 metals on the tissue and 18 metals on the shells of the studied species were presented. Calcium, magnesium and manganese were highly accumulated in the shells of both the species. The absorption level of aluminium, sodium, nickel and lithium was 2.14 ± 0.12 µg/g, 1.40 ± 0.08 µg/g, 0.21 ± 0.4 µg/g, 0.38 ± 0.05 µg/g in *P. fucata.* Among the metals, calcium and iron were highly accumulated in the tissues of both the species and the lower levels of chromium and lithium were also witnessed. In *C. erycina*, the level of lithium, sodium and potassium was 0.43 ± 0.02 µg/g, 2.57 ± 0.09 µg/g and 1.53 ± 0.05 µg/g. In the biota accumulation factor study, for studied species seawater accumulation values (BWAF) were higher than sediment accumulation values (BSAF). The metal pollution index (MPI) was less than 2, which comes under class 1 and is unaffected. Based on the human consumption studies (EDI & THQ) there were some risk factors for children for consuming these species. Additionally, it is important to continuously check the confirmative toxicity of certain metals

found in bivalve species, such as Cd, Pb, and Zn. The amount of toxic metals accumulating in the species under investigation is negligible when compared to the maximum level suggested for human consumption by national and international regulatory agencies.

OP-03

SYNTHESIS AND CHARACTERIZATION OF ALMOND GUM BASED SOLID BIO POLYMER ELECTROLYTE DOPED WITH NH_4SCN

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Abstract

The development of a natural gum based solid polymer electrolyte to move towards a sustainable energy solution gains attention nowadays due to the availability, cost effectiveness, biodegradability, non-toxic nature. Polymer electrolytes made from naturally occurring tree gums such as Guar gum, Tragacanth gum, Agar agar, Arabic gum, are shown to exhibit ionic conductivity suitable for electrochemical applications. In this work, the solid polymer electrolyte membrane is made from almond gum (Amygdalus communis) doped with NH_4SCN salt of various concentrations and its influence on ionic conductivity is studied. The XRD and FTIR analyses validate the structure and the presence of functional groups.

Keywords: almond gum, bio-degradable polymer, structural analysis, ionic conductivity, solution casting.

OP-04

SPECTRAL AND ELECTROCHEMICAL INVESTIGATIONS OF INCLUSION COMPLEX OF 2, 2’-DIHYDROXYBIPHENYL WITH Β-CYCLODEXTRIN AND ITS ANTI-BACTERIAL ACTIVITIES

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Abstract

Inclusion complex of 2,2’-Dihydroxybiphenyl (DHB) with β-cyclodextrin (β-CD) has been investigated by FT-IR, Scanning Electron Microscopy (SEM), XRD, Cyclic Voltammetric method, UV/visible spectroscopy and Fluorescence Spectroscopy. It was testified that the inclusion complex was formed between β-CD and 2,2’-Dihydroxybiphenyl. The formation constant (K) 1:1 stoichiometric of complexation was determined and schematic diagram proposed. FT-IR and SEM analysis confirmed the Solid inclusion and to provide information on the behaviors of DHB inside the cavity of β-CD. It was found that the molecule, one benzene rings entered into the cavity of β-CD. Concerning the structure of the inclusion complex, two –OH groups of DHB in β-CD cavity has been confirmed by Rasmal tool computational analysis. Based on the enhancement of the absorbance and fluorescence intensity of DHB produced through complex formation, a spectrophotometric method for the determination of DHB in bulk aqueous solution in presence of β-CD was developed, which overcome the effect of condition change on the determination of DHB. The Benasi-Hildebrand linear relationship between the absorbance and fluorescence intensity of DHB concentration was prepared in the range of 1 x 10^{-3}M. It shows good anti-bacterial activity against few grams

negative and gram-positive bacteria.

OP-05

ELECTROCHEMICAL REDUCTION OF CO_2 TO VALUE ADDED CHEMICALS USING CU-MODIFIED CONDUCTING POLYMER ELECTRODE

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Abstract:

A viable technique to reduce atmospheric CO_2 concentration and concurrently transform this greenhouse gas into chemicals or fuels with additional value is electrochemical reduction. Electrochemical reduction of carbon dioxide, or CO_2RR, is the process of utilising electrical energy to change carbon dioxideinto more reduced chemical species. Nevertheless, the majority of CO_2 reduction electrocatalysts are powder-based, therefore polymer binders are always needed to make these catalystsfunctional as working electrodes. Catalytic CO_2 reduction has beena popular issue in electrocatalysis research in recent decades. Inelectrocatalytic CO_2 reduction, copper is the sole metal catalyst thatcan produce numerous carbon (C^{2+}) products; nonetheless, thereare still several problems, including inadequate selectivity, significant hydrogen evolution, and poor stability. For Cu-basedcatalysts, a number of synthesis techniques have been established thus far. The electrochemical approach has several advantages over conventional chemical synthesis, including a straight forward procedure, regulated conditions, high safety, and environmental friendliness. The development of CO_2 reduction electrocatalysts and the mechanistic understanding of the CO_2 electro-reductionreaction are the main topics of this article. developments linked toelectrochemical CO_2 reduction in recent years. This study focuses on the use of copper metal in the electrochemical process to minimise CO_2.

OP-06

REMARKABLE SO_2 AND H_2S RESISTANT ABILITY ON CO OXIDATION BY UNIQUE PD/WO_3 3D HOLLOW SPHERE NANOCATALYST: CORRELATING STRUCTURE−ACTIVITY RELATIONSHIPS ON SO_2 EXPOSURE

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Abstract

A simple inorganic route for synthesizing a Pd/WO_3 3D hollow sphere nanocatalyst, where Pd nanoparticles are encapsulated and well distributed on porous tungsten oxide nanospheres. The synthesis protocol has advantages, as it requires no surfactant or stabilizing agent, Pd loading is easily tuned, and the as-synthesized nanomaterials can be directly used as catalysts for the CO oxidation reaction. The synthesized nanocatalyst exhibited 100% CO to CO_2 conversion efficiency at 260 °C. In addition, the nanocatalyst demonstrated remarkable SO_2 (3 ppm) tolerance during the CO oxidation reaction for prolonged SO_2 sulfation of 1−21 h at 260− 400 °C. Moreover, the synthesized nanocatalyst shows H_2S (4 ppm), even in situ H_2S tolerance during the CO oxidation reaction at 260 °C for 1−3 h and exhibited less sensitivity to prolonged and stringent sulfur exposure, with the highest H_2S concentration and maximum 100% CO to CO_2 conversion efficiency obtained after H_2S treatment for the first time based on a Pd-based nanocatalyst to the best of our knowledge. The composition and structure of the R-Pd/WO_3 nanocatalyst were not much influenced, even after the prolonged SO_2 and H_2S exposure during the CO oxidation reaction, as verified from spent catalyst analysis. Finally, our DFT-based model provides insights into understanding the observed sulfur resistance on Pd/WO_3 by analyzing the underlying electronic structure. Therefore, our strategic synthesis

methodology will open up many opportunities to select Pd/metal oxide-based nanomaterials for designing highly efficient, stable, and SO_2/H_2S-resistant nanocomposite catalysts.

OP-07

STUDIES ON POLY(ACRYLATE)S CONTAINING PENDANT LIGAND AND THEIR DIVALENT METAL COMPLEXES DERIVED 2, 4-DIHYDROXY BENZALDEHYDE

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Abstract

A chelating polymer poly (2-hydroxy-4-methacryloyloxy benzaldehyde hydrazone) poly(2H4MBH) was prepared in N, Ndimethylformamide (DMF) at 70^0C using benzoyl peroxide as initiator. Poly (2H4MBH) was characterized by infra-red and 1H-NMR spectroscopic techniques. The molecular weight of the polymer was determined by gel permeation chromatography. Polychelates were obtained when the DMF solution of the polymer containing a few drops of ammonia was treated with the aqueous solution of Cu(II)/Ni(II). Elemental analysis of the polychelates indicates that the metal-ligand ratio was about 1:2. The infrared spectra of polychelates suggest that the metals were coordinated through the oxygen of the phenolic–OH group and nitrogen of the azomethine group. The EPR (Electron paramagnetic resonance) and magnetic moment data indicate a square planar structure for Cu (II) complex whereas octahedral structure for Ni (II) complex. The thermogravimetric analysis, differential calorimetry, and X-ray diffraction data indicated that the incorporation of the metal ions significantly enhanced the degree of crystallinity. The sorption properties of the chelate-forming polymer towards various divalent metal ions Cu (II)

and Ni (II) were studied as a function of pH, nature, and concentration of electrolytes.

Keywords: Methacryloyl chloride, thermal studies, viscosity, chelation properties, regeneration.

OP-08

PREPARATION AND CHARACTERIZATION OF METAL-ORGANIC FRAMEWORK OF COPPER AND 1,3,5-BENZENE TRICARBOXYLIC ACID IN DEEP EUTECTIC SOLVENT OF CHOLINE CHLORIDE AND UREA

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Abstract

Copper 1,3,5-Benzene Tricarboxylic acid metal-organic framework known as $Cu_3(BTC)_2$ (MOF-199 or HKUST-1), is an extremely studied metal-organic framework (MOF) that was first reported in 1999. This MOF is formed from copper ions and benzene-1,3,5-tricarboxylic acid (H_3BTC) and is familiar for its high porosity and specific surface area, which makes it an excellent material for applications such as gas adsorption[1]. The synthesis of $Cu_3(BTC)_2$ can be achieved through various methods. The choice of solvent during synthesis can significantly affect the phase structure, morphology, and specific surface area of the resulting material[1]. Deep eutectic solvents (DES) are composed of a hydrogen bond donor (usually a quaternary ammonium salt or hydrogen bond acceptor) and a hydrogen bond acceptor (often a metal salt or organic compound). DES can be used in the synthesis of metal-organic frameworks (MOFs) to achieve specific properties or enhance their performance. An environmentally benign and energy-efficient process for Cu-Benzene dicarboxylic acid (BDC)

synthesis was developed using choline chloride/urea DES and other DES. Cu-BDC is a promising MOF material with applications in gas storage, catalysis, and adsorption.

In this work Copper and 1,3,5-benzene tricarboxylic acid (BTC) based MOF was prepared in the DES media of Choline chloride (ChCl) and Urea (U). Proton NMR, SEM, EDAX and other techniques characterized the Cu-BTC MOF prepared by this method.

OP-09

SYNTHESIS, STRUCTURAL, OPTICAL, THERMAL, HIRSHFELD SURFACE ANALYSIS AND ANTIBACTERIAL INVESTIGATIONS OF BIS (2-AMINOBENZTHIAZOLINIUM) TETRABROMOZINCATE (II) MONOHYDRATE

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Abstract

Bis(2-aminobenzthiazolinium) tetrabromozincate (II) monohydrate crystal was produced by the slow evaporation of solution technique (SEST) at room temperature and their triclinic structure was determined using single-crystal X-ray diffraction (XRD). FT-IR spectral analysis demonstrated the presence of protonated NH group symmetric stretching frequencies at 3153 Cm^{-1}. The diffuse reflectance spectrum of compound increased above 235nm. The absorption was primarily due to the transitions within the organic part of the hybrid and charge transfer. The compounds exhibit solid-state fluorescence at room temperature consistent with photoluminescence investigations. The thermal stability of the compounds is up to 260 °C according to TG-DTA study. The CSM calculation of SnX_6^{2-} (X=Cl, Br) closely aligns with the ideal tetrahedral geometry of the anions. Hirshfeld surface analysis which is obtained from single-crystal XRD data is used to investigate the intermolecular interactions and crystal

packing and exposes stronger contacts associated with strong interactions. The antibacterial studies of the investigated compounds were comprehensively examined against pathogens including *Enterococcus faecalis, Streptococcus pyogenes, Pseudomonas aeruginosa,* and *Proteus mirabilis* by using agar well diffusion method. The results indicate significant efficacy in inhibiting bacterial growth for the compounds.

OP-10

SYNTHESIS, SPECTRAL, SINGLE CRYSTAL XRD, HIRSHFELD SURFACE ANALYSIS AND DFT STUDIES OF A NEW SALEN TYPE SCHIFF BASE DERIVATIVE

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Abstract

A new 5-Bromosalicylaldehyde derived Salen Schiff Base derivative was synthesized and characterized by spectral and SC-XRD studies. The salen moiety adopts an E configuration with the isopropyl (C-3) and Phenyl (C-4) substituents. The geometry of the molecule was optimized by DFT using the B3LYP/6–31++G(d,p) level basis set. Comparison of calculated geometrical parameters with the experimental SC-XRD results revealed that they are in good agreement. The HOMO and LUMO energies, chemical reactivity parameters and molecular electrostatic potential were also computed. Hirshfeld surface analysis and two-dimensional fingerprint plots revealed the nature of intermolecular interactions exist in the crystal structure. Molecular docking study was performed to investigate the binding affinity of the title ligand with the human oestrogen receptor alpha (hER alpha) protein (PDB Code: 3ERT).

Keywords: Schiff Base, NMR, Single Crystal XRD, DFT, and Molecular docking.

OP-11

ORGANIC THIOCYANATE FUSED HETEROCYCLE: SYNTHESIS, STRUCTURAL, HIRSHFELD SURFACE, ENERGY FRAMEWORK, DFT AND IN-SILICO MOLECULAR DOCKING STUDIES

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Abstract

An organic thiocyanate derivative synthesized by adopting a multi-step synthetic strategy. The crystal structure of the compound was established by Single-crystal XRD analysis. The compound crystallizes in a triclinic crystal system with the space group $P\bar{1}$. Its unit cell parameters were a = 9.3404 (6) Å, b = 13.1888 (9) Å, c = 17.4549 (11) Å, α = 79.515 (2)°, β = 87.981 (2)°, γ = 88.516 (2)° and Z=4. The optimized structure with its bonding aspects has been examined utilizing the DFT-B3LYP technique with a basis set 6-311++G(d,p). In addition, Mulliken population, HOMO-LUMO, and MEP analysis have also been executed. The Hirshfeld surface and 2D fingerprint plot were generated using *Crystal Explorer 21.0*. The molecular packing was visualized in terms of dispersion, electrostatic, and total energies using three-dimensional Energy Framework analysis. Furthermore, Molecular docking with breast cancer protein (3*ERT*) was carried out using AutoDock4 software. The docking study reveals appreciable binding affinity (-9.11 kcal mol^{-1}) and the interaction of ligand with amino acid residues.

Keywords: Organic thiocyanate, Piperidin-4-one, DFT, Hirshfeld analysis, Molecular Docking

OP-12

EFFECT OF CARBONATE CYCLE ON THE CACO3 SCALE DEPOSITION ON THE SURFACE OF COPPER METAL IN THE PRESENCE OF MAGNESIUM IONS AND THE IMPACT OF SHAPE, SIZE, AND SURFACE AREA OF CONTACT UNDER EDTA INFLUENCE AT 60^{O}C

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Abstract

The deposition of calcium carbonate ($CaCO_3$) from its sludge was studied on copper substrate. Ethylenediaminetetraacetic acid was used as a chelating agent with carbonate ions and tested for its influence on the deposition. The experiments were carried out at 60°C° for 15 days with a 10-hour daily heating interval. and the effect of direct heating and indirect heating was studied. The samples were characterized by XRD, FTIR, and Fe- SEM techniques. The data revealed that the complex forming nature of EDTA, the shape of the crystallite, and the area of contact are the key factors for the deposition of CaCO3 on metal surfaces.

Keywords: Internal water treatment, scale inhibitors, morphology, polymorphism.

OP-13

SILVER DOPED ZINC STANNATE (AG-$ZnSnO_3$) NANOCOMPOSITE FOR EFFICIENT PHOTOCATALYTIC DEGRADATION OF TEXTILE DYE

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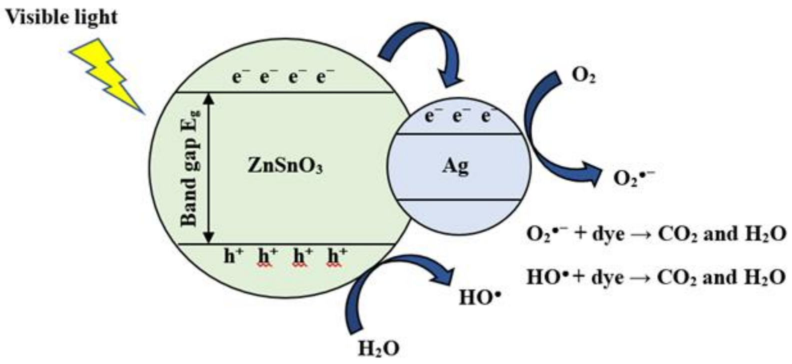
Abstract

All living things are adversely affected by untreated dye effluents from textile factories, which are one of the main causes of water pollution. More effectively than the currently used conventional approaches, photocatalytic activity using $ZnSnO_{3-}$ facilitates the degradation of organic contaminants. $ZnSnO_3$ absorbs only UV light due to its large bandgap which leads to low degradation yield. Therefore, in this work pure and Ag-doped $ZnSnO_3$ nanocomposites were prepared by biosynthesis method. The structural analysis confirms the orthorhombic perovskite structure of $ZnSnO_3$ and the crystalline size was found to be 9nm. From the optical analysis, there is a redshift of absorbance edge for Ag-doped $ZnSnO_3$ over the pure $ZnSnO_3$ and the bandgap was found to be 2.79 eV. The morphological analysis shows that the samples are spherical. The presence of Zn-O and Sn-O functional groups was established by FTIR analysis. The XPS analysis confirms the chemical composition and binding energy of Ag-doped $ZnSnO_3$. For the photocatalytic activity, crystal violet (CV) dye was taken as a model pollutant. The modification of $ZnSnO_3$ using Ag-doping can further enhance the photocatalytic activity due to its low bandgap and larger surface area. Overall, Ag-doped $ZnSnO_3$ nanocomposite can serve as a highly efficient photocatalyst to treat wastewater for environmental remediation.



OP-14

PREPARATION OF MAGNESIUM FERRITE NANOPARTICLES WITH VISIBLE LIGHT ENHANCED PHOTOCATALYTIC ACTIVITY FOR MALACHITE GREEN DYE DEGRADATION

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Abstract

Magnesium ferrite ($MgFe_2O_4$) nanoparticles have attracted extensive interest in various industrial fields with unique physical and chemical properties. Photocatalytic activity has emerged as an eco-friendly technique for removing dye contaminants in wastewater treatment. In this work, $MgFe_2O_4$ nanoparticles were synthesized by green synthesis using *Erythrina variegata* leaf extract as a stabilizing and reducing agent for photocatalytic activity. The prepared $MgFe_2O_4$ nanoparticles were studied through PXRD, FTIR, UV-visible spectroscopy, and SEM with EDX to confirm the structural, optical, morphological, and compositional studies. The cubic structure of $MgFe_2O_4$ nanoparticles is confirmed by PXRD with a calculated average crystalline size is 26 nm. In the FTIR spectra, the strong relevant peaks of $MgFe_2O_4$ NPs showed Fe-O (tetrahedral site) band at 596 cm^{-1}, and bands at 421 cm^{-1} were assigned to the stretching modes of Mg-O (octahedral site), respectively. The optical investigation revealed that $MgFe_2O_4$ nanoparticles have a band gap of about ~1.8 eV using UV-visible spectroscopy. The SEM images showed the agglomerated particles due to magnetic interactions and the EDX confirms the elemental compositions such as Mg, Fe, and O present in the $MgFe_2O_4$ nanoparticles. The photocatalytic performance of prepared $MgFe_2O_4$ nanoparticles showed efficient degradation of malachite green (MG) dye under visible light irradiation

with 90% degradation achieved within 60 mins.

OP-15

SYNTHESIS, SPECTRAL, SC-XRD, DFT AND BIOLOGICAL EVALUATION OF PROPARGYL PIPERIDIN-4-ONE DERIVATIVE

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Abstract

The title compound has been synthesized by the reaction of 3,5-dimethyl 2,6-diphenylpiperidin-4-one with propargyl bromide using potassium carbonate as catalyst in dry DMF. Structural elucidation of the title compound has been carried out by IR and NMR techniques. Further, structure of the title compound has been evaluated by single crystal X-ray diffraction technique. Single crystal of the title compound has been grown by slow evaporation method from ethanolic solution. The title compound has been crystallized in monoclinic crystal system and the unit cell parameters are a = 11.4947(11) Å, b = 11.3772(11) Å, c = 14.9114(15) Å, $\alpha = 90°$, $\beta = 108.235(4)$ °, $\gamma = 90°$. Single crystal XRD study reveals that piperidone ring adopts chair conformation with equatorial orientation of methyl and phenyl group. The molecular structure of the title compound has been optimized using density functional theory (DFT) at B3LYP/6–311 G (d, p) level and the results compared with the experimental results. The Hirshfeld surfaces and 2D fingerprint plots were generated using *CrystalExplorer 21.0.* Two-dimensional fingerprint plots disclose the occurrence of all inter-molecular contacts exist in the crystal. The total interaction energy of the title compound has been calculated for a 3.8 Å radius cluster of molecules around the selected molecule. Docking study has been carried out for the synthesised compound using proteins (PDB Code: 3*ERT*).

Keywords: N-Propargyl derivative, SC-XRD, Chair conformation, DFT and Molecular docking.

OP-16

INTERFACIAL ELECTRON BOOSTING AND MAGNETICALLY RELEASABLE Fe_3O_4@MnO_2 CYLINDRICAL NANOTUBES FOR THE CATALYTIC REDUCTION OF EOSIN -Y DYE DECOMPOSITION

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Abstract

Fe_3O_4@MnO_2 NCs as a heterogeneous catalyst were synthesized by biogenic conversion route. Thus, biogenic heterocatalyst were confirmed various analytical tools such as XRD, SEM EDX, TEM/HRTEM, BET isotherm spectroscopic studies. The double phase nanocatalyst was confirmed by an X-Ray Diffraction analysis. The globular form of the integrated nanocomposite was revealed using scanning electron microscopes. The magnetic features have been inspected using a vibrating sample magnetometer. The catalysts in dispute does have a more extensive contact region is also asymmetrical,as shown by atomic force microscope. The developed heterogenous catalyst were further tested for their catalytic performance in removing Eosin - Y dye. Within 20 minutes, as the derived Fe_3O_4@MnO_2 NCs nanorods completely decolorized almost 99.9 percent of the Eosin - Y dye. Cleaner and more efficient nanorods for contaminant remediation were developed, and greener synthesis for metallic nanoparticles was consistently demonstrated. This investigation demonstrates

the greensynthesis of $Fe_3O_4@MnO_2$ heterogeneous catalyst and its applications in environmental remediation.

OP-17

PYTO-CONSTITUTIONS OF $CU@FE_3O_4$ NANO CUBE FOR MALACHITE GREEN DYE DEGRADATIONS USING PHOTO CATALYSIS APPROACH

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Abstract

This investigation explains the in-situ green synthesis of a magnetic nano catalyst consisting of Cu/Fe_3O_4 using the extract from the flowers of the Moringa oleifera plant. No stabilizers or surfactants were used in the process, and it was carried out in an environmentally friendly manner. In order to analyze the catalyst, a variety of techniques such as XRD, SEM, EDS, UV–visible, TEM, VSM, and TGA were used. According to the results of Fourier transform infrared spectroscopy, the C=O and C-O groups in the plant seeds extract are very important for shielding the nanoparticles from the outside environment. The produced nanocatalyst was used to decrease Malachite Green (MG) at room temperature, and the performance of the nanocatalyst as a catalytic agent was analyzed. To extract the catalyst, an external magnet was employed, and despite its several applications, there has been no noticeable decline in the level of effectiveness it has as a catalyst. In addition, the recycled Cu/Fe3O4 magnetic nanocatalyst seems to be stable, according to data derived from XRD patterns and FT-IR spectroscopy.

Keywords Cu/Fe3O4 · Malachite Green · Nanocatalyst · BET

OP-18

ACENAPHTHO-IMIDAZOLE BASED "TURN ON" CHEMOSENSORS FOR SELECTIVE DETECTION OF TIN AND COPPER IONS AND THEIR BIO-IMAGING APPLICATION

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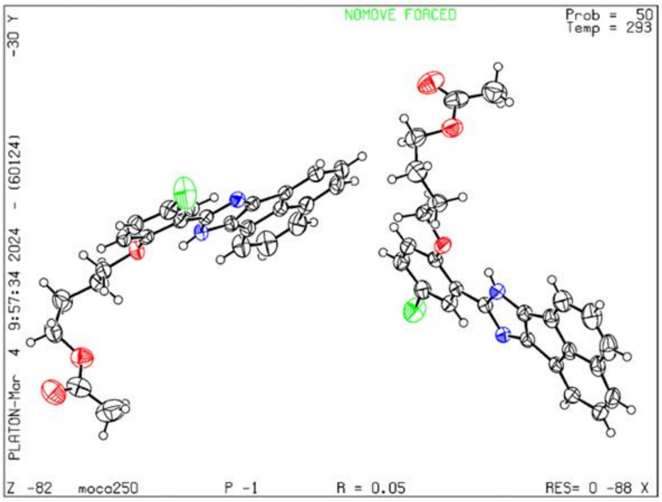
Abstract

In this study, we have synthesized two acenaphtho-imidazole-based chemosensors 4-(2-(7H-acenaphtho[1,2-d] imidazole-8-yl)-4-bromophenoxy) butylacetate (**1**) and 4-(1-(7H-acenaphtho[1,2-d] imidazole-8-yl) naphthalen-2-yloxy) butylacetate (**2**) for the detection of Tin (Sn^{2+}) and Copper (Cu^{2+}) ions. The compounds were thoroughly characterized using various spectroscopic techniques including FT-IR, ^{1}H NMR, ^{13}C NMR, Mass Spectrometry, and single crystal X-ray diffraction analysis. Chemosensors **1** and **2** exhibited "Turn On" fluorescence response at 570 nm and 615 nm, respectively, in the presence of Sn^{2+}/Cu^{2+} ions, owing to the chelation enhanced fluorescence (CHEF) mechanism. Binding constants for the formation of **1**+Sn^{2+} and **2**+Cu^{2+} complexes were determined to be approximately 1.6×10^{4} M^{-1} and 3.3×10^{4} M^{-1}, respectively, and Job's plot confirmed a 1:1 stoichiometry between chemosensors and Sn^{2+}/ Cu^{2+} ions. Additionally, the detection limits for Sn^{2+}/ Cu^{2+} ions were determined to be 1.2×10^{-9} M and 2.1×10^{-9} M for chemosensors **1** and **2**, respectively. Furthermore, the applicability of chemosensors **1** and **2** for live cell imaging was demonstrated, revealing negligible cytotoxicity and promising prospects for cellular detection of Sn^{2+}/ Cu^{2+} ions.



OP-19

GADOLINIUM DOPED SMART IRON OXIDE NANOPARTICLES FOR THERANOSTIC APPLICATIONS

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Abstract

Superparamagnetic Iron oxide nanoparticles (SPIONs) have been investigated as the highly systemic material with favourable size and tuneable magnetic properties for Magnetic Resonance Imaging (MRI) and targeted drug delivery. In this study, Gd doped SPIONs structure were designed which was encapsulated with biodegradable polymers using coprecipitation method. Furthermore, the biomedical application of this core structure is enhanced by combining Cisplatin (Cis) for targeted drug delivery to monitor in-vivo cancer treatment. The effects of different parameters on adsorption capacity, such as pH, acid concentration, the type and amount of adsorbent, and contact and ultrasonication times were optimized under optimum conditions. The structure and different properties of the synthesized

SPIONs-Gd-Cis were investigated using Fourier Transform Infrared Spectroscopy (FT-IR), XRay Diffraction (XRD), Field emission-scanning electron microscopy (FE-SEM), transmission electron microscope (TEM), Dynamic light scattering (DLS), and a Vibrating Sample Magnetometer (VSM). The results confirmed the successful preparation of magnetite nanocomposite and anchoring of Fe3O4 nanoparticles with size of 12nm in average and efficient drug loading capacity. In case of MRI, high performance with T1 and T2 magnetic relaxation rate was achieved for effective signalling. Additionally, cytotoxicity studies were investigated with in-vitro and in-vivo studies using cancer cell lines. Thus, the synthesized core SPIONs structures has the potential significance in both MRI and assessment of drug targeting.

Keywords: SPION, MRI, Drug targeting, Cis, Magnetic relaxation

OP-20

2,3-DIPHENYL-2,3-DIHYDROQUINAZOLINE-4(1H)-ONE AS A POTENT INHIBITOR OF BCL-2 FAMILY PROTEINS FOR TARGETING U-87 GLIOBLASTOMA: SYNTHESIS, DFT CALCULATIONS, MOLECULAR DOCKING STUDIES, AND MTT ASSAY

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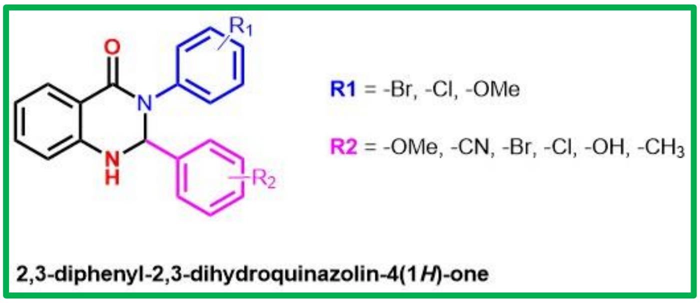
Abstract

Glioblastoma is the most common and destructive type of brain tumour, with increasing complexity. As current treatment methods for malignant glioma, such as radiotherapy and chemotherapy, are not effective, the development of novel therapeutic compounds is necessary.

In this study, we investigated the inhibitory effect of 2,3-diphenyl-2,3-dihydroquinazoline-4(1H)-1-one on the proliferation of human glioma U87 cells using an MTT assay to assess cell viability in vitro. 2,3-Diphenyl-2,3-dihydroquinazoline-4(1H)-1-one derivatives are considered as broad-spectrum cyto toxic agents. Further, molecular docking study and DFT studies were conducted to better understand the interactions between the most active compounds and Bcl-2 family proteins. Moreover, an ADME/T analysis was performed for the most active compounds. A unique multicomponent one-pot green synthetic method was used to synthesize 2,3-diphenyl-2,3-dihydroquinazoline-4(1H)-1-one derivatives. To generate geometric optimization parameters, MEP analysis, and HUMO-LUMO quantum parameters of the synthesized molecules. The in vitro analysis revealed the promising inhibitory activity of the synthesized molecules and could be considered as a lead compound for malignant glioma DFT/B3LYP theory and the def2-TZVP basis set were used.



2,3-diphenyl-2,3-dihydroquinazolin-4(1*H*)-one

- ❖ **Organo-Catalyst**
- ❖ **One-Pot Reaction**
- ❖ **Green Solvent**
- ❖ **Chromatography- Free**
- ❖ **Druggable nature**
- ❖ **Feasible condition**

OP-21

WATER DRIVEN REVERSIBLE NITRO QUINOLINE D-Π-A AZINE SYSTEM FOR SPOTTING CHEMICAL WARFARE AGENTS (CWAs)

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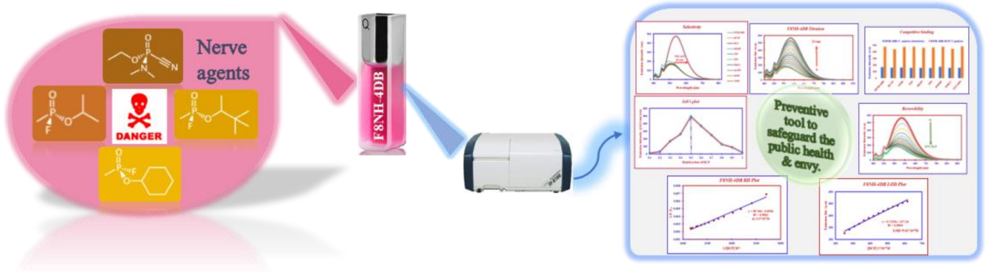
Abstract

The toxicological nature of chemical warfare agents (CWAs) brings about

incapacitating effects on living beings or else in severe cases leads to lethal. Unlike explosives and military farm, CWAs are relatively easy to cause direct impact on health and well-being of humans and to the environment. The initiatory to spotlight such CWAs, numerous sensor modalities like optical, electrochemical, mass-spectrometry and nanotech based motifs have been developed and showcasing their potency towards the detection of CWAs. Recently emphasis to designing the optical sensors, with trends like miniaturization, multiplexing, and integration into compact devices holding effective selectivity, sensitivity and field deployability is focussed to address this challenge[1-5]. In order to easy identify CWAs, we developed the D-**π**-A azine based motif Nitro-Quinoline system called 4-((*E*)-((*E*)-((4-chloro-8-nitro-1,2-dihydroquinolin-3-yl) methylene) hydrazono) methyl)-*N*, *N*-diethylaniline (NQH). Further incorporated the detailed emission behaviour of NQH towards various Organophosphates and phosphonates.

Remarkably, the synthesized nitro-quinoline chemosensor NQH exhibited optical selectivity and sensitivity in favouring the detection of one among the nerve agent mimics diethyl chlorophosphate (DCP). A Significant LOD value was exhibited by the newly synthesised nitro quinoline sensor observed as 5.01 x 10^{-6}M. More interestingly the reversibility of the DCP detecting effect upon the addition of water could lead to practical usability of NQH in real sample analysis for identifying the presence of CWAs. Further, the nitro-quinoline chemosensor NQH in this work could contribute to safeguard the public health and environment preventively.



OP-22

MONITORING SOLAR THERMAL PERFORMANCE THROUGH ADVANCED TEMPERATURE SENSING AND LOGGING SYSTEM

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Abstract

Monitoring solar thermal systems over long periods traditionally requires substantial manual effort due to the limitations of conventional thermometers, particularly their inability to log temperature data digitally. To overcome these challenges, we have developed a sophisticated prototype leveraging Raspberry Pi single-board computers and advanced temperature sensors. This innovative approach simplifies the monitoring process and introduces digital logging capabilities, revolutionizing temperature measurement in solar thermal systems. Our work introduces the performance capabilities of the Raspberry Pi and sensor-based Temperature Measuring and Logging System, specifically designed for solar thermal applications. This automated prototype guarantees consistent and reliable temperature logging over prolonged periods, a significant advancement over traditional methods. We achieved this through the creation of computational programming code written in Python, which not only facilitates precise measurement and logging but also enhances the system's efficiency and accuracy.

The use of this Linux OS-based single-board computer (Raspberry Pi) enables the storage of logged data on the cloud, ensuring data is easily accessible and secure. This feature is particularly beneficial for long-term studies and monitoring, where data integrity and availability are paramount. The potential applications of this prototype are vast, extending its utility to real-time solar thermal experiments. Its ability to provide autonomous and efficient

temperature monitoring shows its potential as a transformative tool in the field. This research significantly contributes to the exploration of sustainable energy solutions, offering a reliable, adaptable, and innovative tool for temperature measurement and monitoring in solar thermal experiments. Furthermore, the implications of this system extend beyond solar thermal applications, presenting opportunities for its integration into a wide range of renewable energy studies and environmental monitoring projects. The flexibility and scalability of the prototype make it an ideal candidate for adapting to various experimental setups and research needs.

OP-23

FLUORESCENCE TURN-ON DETECTION OF CHLORTETRACYCLINE ANTIBIOTICS USING WS_2 QUANTUM DOTS

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Abstract

Chlortetracycline (CTC) is a broad-spectrum antibiotic widely used in animal husbandry for treating various diseases and also provokes animal growth rate. Regular ingestion of CTC will result in drug residues in animal products such as milk, meat, and eggs. Hence, monitoring of CTC in food and water samples is highly essential. In this work, we systematically investigated the fluorescence behavior of the CTC antibiotics in both acidic and alkaline mediums. In various pH ranges from pH 2 to pH 12, the fluorescent behaviour of CTC was observed in an alkaline medium. In alkaline conditions, the conversion of hydroquinone (HQ) occurs when OH^- ions replace chlorine in the CTC structure. UV-absorbance analysis confirms the CTC-HQ conversion. Under optimal pH CTC, the fluorescence response ranged from 0.15 µM to 10 µM, with a limit of detection of 0.06 µM. Further to improve the sensitivity of CTC detection, we developed a stable photoluminescence fluorophore (WS_2 QDs) by a

simple hydrothermal technique. HR-TEM studies indicate the formation of WS_2 QDs with an average size of 4 nm. it exhibits a wider detection range (0.01 µM to 10 µM) and a detection limit of 0.026 µM, leading to higher sensitivity than CTC fluorescence. Interestingly, the suggested WS_2 QDs material displayed high selectivity by distinguishing CTC from other tetracycline group compounds such as OTC and TC. Furthermore, we successfully conducted CTC detection in real samples such as water, soil extract, milk, and chicken and found excellent recoveries.

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OP-24

SYNTHESIS, SPECTRAL AND STRUCTURAL STUDIES ON BIS(N-DODECYL-N-(4-FLUOROBENZYL) DITHIOCARBAMATO-S, S') COPPER(II)

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Abstract

Bis(N-dodecyl-N-(4-fluorobenzyl) dithiocarbamato-S, S') copper (II) has been prepared and characterized using IR and UV-Visible spectroscopy. Structure of the complex was determined using single crystal X-ray crystallography. In this complex the copper atom is situated on a centre of symmetry and the asymmetry unit consists of one half of a molecule.

The coordination geometry around the copper (II) ion in the complex is a distorted square planar geometry. The geometry around copper (II) is distorted as a consequence of the restricting chelating angle of the dithiocarbamate ligand (S-Cu-S=77.67(17)°). The study of single crystal X-ray diifraction shows that C-H···S interactions among molecules of complex participate in cooperative way to stabilize supramolecular interactions. Hirshfeld surface analysis of complex revealed that the most important interaction is the H···H contact.

OP-25

HYDROTHERMAL SYNTHESIS OF BIMETAL OXIDE/2D MATERIAL COMPOSITES FOR SUPERCAPACITOR APPLICATION

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Abstract

Hydrothermal synthesis offers a versatile approach for tailoring $NiMoO_4$ materials optimized for supercapacitor application. This method involved dissolving precursor salts, comprising nickel and molybdenum compounds in water. By adjusting synthesis ratios, the stoichiometry of the resultant $NiMoO_4$ material was tested for supercapacitor. Structural and morphological characterization techniques were employed to validate the $NiMoO_4$ material. The resistance of materials was analysed by Electrochemical Impedance Spectroscopy (EIS). The supercapacitance behaviour of $NiMoO_4$/2D materials was examined by cyclic voltammetry and charge-discharge studies. This abstract highlight the significance of synthesis ratio optimization in hydrothermal synthesis, offering insights into how controlled variations

can tailor $NiMoO_4$ for improved supercapacitor functionality.

Keywords: Hydrothermal synthesis, $NiMoO_4$, Supercapacitors, Charge-discharge studies

OP-26

SYNTHESIS, STRUCTURE AND COMPUTATIONAL STUDIES OF A NEW *TRANS*-DIAQUABIS(1,2-DIAMINO-1-PHENYLPROPANE-*Κ*^{2}N,*N′*)NICKEL(II)CHLORIDE DIHYDRATE COMPLEX

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Abstract

Unsymmetrically substituted vicinal diamines have a wide range of applications in the synthetic and medicinal fields. Also, these are capable of co-coordinating with many metals to form their complexes. Furthermore, these metal complexes being analogues of *cis*-platin attracts huge biological interests and also, these complexes find extensive applications in the material field as well. One such new bio-active unsymmetrically substituted vicinal diamine nickel complex *viz.*, *trans*-Diaquabis (1,2-diamino-1-phenylpropane-κ^{2}N, N′) nickel (II) chloride dihydrate have been synthesized. The synthesized complex structure has been confirmed by FT-IR, ESI-mass, UV-Vis, ^{1}H NMR and SC-XRD [CCDC: 2210342] studies. The compound crystallized in monoclinic crystal system with the P21/c Space group. The unit cell parameters area = 12.1130(7) Å, b = 7.3062(4) Å, c = 14.0441(8) Å, α = 90°, β = 91.589°, γ = 90. Hirshfeld surface analysis has been done using *CrystalExplorer21.5* software to understand the structural features & interactions at the molecular level and also, its docking affinities towards human estrogen receptor (hER alpha) 3ERT protein have been identified using *Autodock 4.1* software. The compound showed a good docking score of -8.50 kcal/mol^{-1}, which is quite comparable with that of a POM drug *viz.*, doxorubicin.

Keywords: Vicinal diamine complex, Nickel(II) complex, Cheminformatics of Ni(II) complex, Hirshfeld surface and docking studies of vicinal diamine complex.

OP-27

BISPHENOL-A SENSING AND QUANTIFICATION IN PACKED FOOD AND BAKERY PRODUCTS

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Abstract

This research aims to address the increasing demand for a sensitive, rapid, and cost-effective detection system for the synthetic compound Bisphenol A (BPA). BPA's widespread use in various food packages raises concerns about human health risks. The research involves the need for sustainable and bio-inspired alternatives for the detection of BPA, considering the challenges associated with interference, detection limits, effect of pH and sensor stability. The aim is to develop and optimize polyphenylalanine-modified electrodes for more effective BPA sensing, elucidating the molecular structure and electrochemical behavior of the conductive polymer. The methodology involves the synthesis of polyphenylalanine through oxidative electropolymerization of phenylalanine monomers on a Glassy Carbon Electrode (GCE), with subsequent characterization using SEM, FT-IR, XRD, and XPS. Under the optimum conditions of pH 3.0, the sensor showed a linear range with a low detection limit of 0.16µM.

Keywords: Bisphenol A, Polyphenylalanine, Electrochemical sensing, Modified electrodes, Environmental monitoring, Sensor stability.

OP-28

SPECIATION STUDIES OF TERNARY COMPLEXES OF CO(II), NI(II), CU(II) AND ZN(II) WITH MERCAPTOSUCCINIC ACID AND L-CYSTEINE IN ETHYLENE GLYCOL-WATER MIXTURES

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Abstract

Interaction of Co(II), Ni(II), Cu(II) and Zn(II) metal ions with Mercaptosuccinic acid and L-Cystein have been studied pH-metrically at an ionic strength of 0.16 mol L^{-1} and at a temperature of 303.0 K in EG-water mixtures. The stability constants of ternary complexes were calculated using the pH-metric data. Best fit chemical models representing the metal complexes with different compositions were obtained using MINIQUAD75 computer program. Mononuclear complexes of the type MLX and MLX_2 where M=Co(II), Ni(II), Cu(II) or Zn(II), L=MSA and X=Cys were found to exist in EG-water mixtures. The results show that the stabilities of ternary complexes in EG-water mixtures are more than in aqueous medium, Further, the trend of the variation in the stability constants with changing dielectric constant of the medium is explained based on the electrostatic and non-electrostatic interactions of the side chains of the ligands, charge neutralization and chelate effect. Species distribution diagrams were generated using HYSS program. Distribution diagrams with pH at different compositions of EG and structures of plausible ternary complexes are also presented.

Keywords: Mixed-ligand complexes; MSA, Cys; EG, pH metric studies; Stability constants

OP-29

STUDIES ON POLY(ACRYLATE)S CONTAINING PENDANT LIGAND AND THEIR DIVALENT METAL COMPLEXES DERIVED 2, 4-DIHYDROXY BENZALDEHYDE

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Abstract

A chelating polymer poly(2-hydroxy-4-methacryloyloxy benzaldehyde hydrazone) poly(2H4MBH) was prepared in N,Ndimethylformamide (DMF) at 70^0C using benzoyl peroxide as initiator. Poly (2H4MBH) was characterized by infra-red and 1H-NMR spectroscopic techniques. The molecular weight of the polymer was determined by gel permeation chromatography. Polychelates were obtained when the DMF solution of the polymer containing a few drops of ammonia was treated with the aqueous solution of Cu(II)/Ni(II). Elemental analysis of the polychelates indicates that the metal-ligand ratio was about 1:2. The infrared spectra of polychelates suggest that the metals were coordinated through the oxygen of the phenolic–OH group and nitrogen of the azomethine group. The EPR (Electron paramagnetic resonance) and magnetic moment data indicate a square planar structure for Cu(II) complex whereas octahedral structure for Ni(II) complex. The thermogravimetric analysis, differential calorimetry, and X-ray diffraction data indicated that the incorporation of the metal ions significantly enhanced the degree of crystallinity. The sorption properties of the chelate-forming polymer towards various divalent metal ions Cu(II) and Ni(II) were studied as a function of pH, nature, and concentration of electrolytes.

Keywords: Methacryloyl chloride, thermal studies, viscosity, chelation properties,

regeneration

OP-30

ULTRASOUND ASSISTED ONE-POT MULTICOMPONENT SYNTHESIS OF PYRANOPYRAZOLES BY HETEROGENEOUS MCM-41@SILANE ANCHORED SCHIFF BASE METAL COMPLEX

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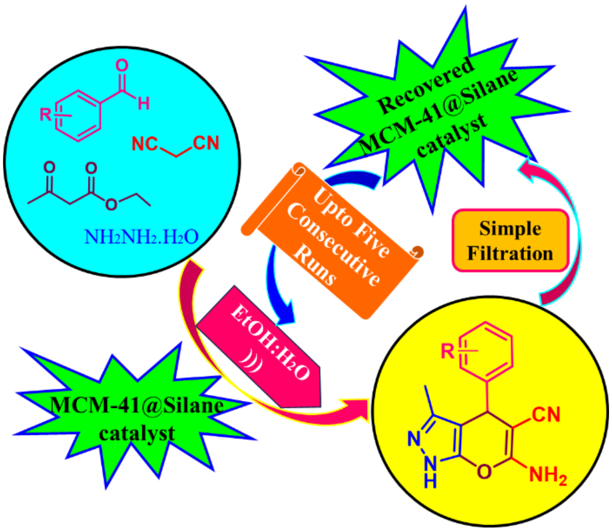
Abstract

A new class of copper schiff base complex of mixed ligands was implanted on MCM-41 to form a simple, reusable heterogeneous catalyst. The synthesized mesoporous material has been characterized by FT-IR, PXRD, SEM, EDX, ICP-OES and TGA analysis. Catalytic performance of our mesoporous metal complex on ultrasonic synthesis of pyranopyrazole from ethylacetoacetate, malononitrile, hydrazine hydrate with variety of aryl aldehydes was studied. Good to high yield of pyranopyrazole analogue was prepared using low cost, highly efficient and reusable catalyst by simple one-pot multi-component experimental procedure in short reaction time which makes more advantage of sustainable chemistry. In addition, Hot filtration test has also been carried out for the finding of metal leaching and the existence of heterogeneous nature of the synthesized catalyst even after five cycles.

Keywords: Heterogeneous catalyst, MCM-41, Multicomponent, Mixed ligands, Ultrasonication



OP-31

A NOVEL CLASS OF Ru (II) HETEROCYCLIC HYDRAZONE COMPLEXES FOR N-ALKYLATION OF AMINES AND ANTIBACTERIAL ACTIVITIES

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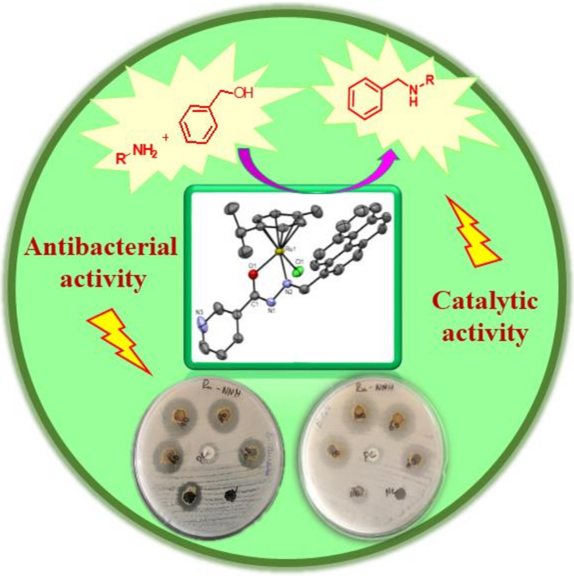
Abstract

A novel class of Ruthenium (II) half-sandwich heterocyclic hydrazone complexes have been successfully synthesized. The Ru(II) complexes were characterized by UV-Vis, FT-IR, NMR and Mass spectral techniques. The solid-state structure of Ligands and Complexes was determined by Single Crystal X-ray diffraction method. Further, the complexes were utilized for catalytic and anti-bacterial activity. The catalytic efficiency of these Ruthenium complexes in the synthesis of N-alkylation of amines was explored and critically analysed. The antibacterial activity of the complexes was also studied against both Gram-positive (*Staphylococcus aureus* & *Enterococcus faecalis*) and Gram-negative (*Klebsiella pneumoniae* & *Escherichia coli*). These two different studies demonstrate the wide scope of catalytic and

biological importance of our newly prepared Ruthenium catalyst.

Keywords: Ruthenium complex, N-alkylation, Anti-bacterial activity



OP-32

Improving the electrocatalytic property of Layer Double Hydroxide by 5d transition metal doping for highly efficient water oxidation reaction

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Abstract

The depletion of fossil fuels and the rise in environmental problems limit the expansion of the world economy. The creation of a sustainable and environmentally beneficial method for producing energy has the ability to resolve resource, energy, and environmental conflicts. Hydrogen has been shown to be a promising alternative energy source because of its high specific energy density to replace carbon-based fuels. Using electrochemical water splitting to separate water molecules into molecular hydrogen and oxygen, is the safest, most efficient, and most environmentally friendly approach to produce electricity. It comprises two half-cell reactions namely Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER). Comparatively, the Oxygen Evolution Reaction (OER) has poor efficiency which serves as a barrier to the water splitting process. Because of its distinct reaction mechanism, OER is kinetically slow and often proceeds at high overpotential. The creation of high-performance electrocatalyst is a very effective way to improve poor kinetic behaviour of the oxygen evolution reaction (OER). Here, we synthesised Tungsten doped NiCo-LDH through Hydrothermal method for highly efficient OER activity. To achieve a current density of 50 mA cm^{-2}, the catalyst 0.12mmol W doped NiCo–LDH/NF requires overpotential value of 260 mV and Tafel slope value of 62.64 mV dec^{-1} respectively. Additionally, the synthesised 0.12mmol W doped NiCo-LDH/NF exhibit strong stability over a longer duration of 46 hours at 1.66 V vs RHE.

Key Words: Metal doping, Layer Double Hydroxides, Hydrothermal method, Water oxidation reaction.

OP-33

COW DUNG BIOMETHANE POTENTIAL TEST BY USING AMPTS-11 INSTRUMENT

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Abstract

Biogas is a renewable energy source produced through the anaerobic digestion of organic matter such as agricultural waste, food scraps, sewage sludge, and animal manure. Anaerobic digestion is a natural biological process where microorganisms break down organic material in the absence of oxygen, resulting in the production of biogas. The production of biogas offers several environmental and economic benefits, including reducing greenhouse gas emissions, providing a renewable energy source, and managing organic waste effectively. Cow dung, a readily available organic material rich in organic matter and nutrients, serves as an excellent feedstock for anaerobic digestion, a natural process facilitated by microbial activity in the absence of oxygen. In this work using a cow dung for biogas production to be tested by AMPTS-11 instrument. 1:3 and 1:1 ratio of Cow Dung with Different Volumes (1800 mL, 1400 mL, 1000 mL and 400 mL) was tested the biogas production. The results showed 1800 mL of 1:1 ratio of Cow Dung obtained higher gas production of 7,521 NmL compared with 1:3 ratio of Cow Dung (2,678 NmL)

Keywords: AMPTS-11 (Automatic Methane Potential Testing System), Cow Dung, Renewable energy Source

OP-34

STUDY ON SYSTEMATIC ADSORPTION EFFICIENCY OF POROUS Zn-BiMOFs AGAINST AGRICULTURAL PESTICIDE AND ITS KINETIC PROPERTIES

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Abstract

Around the world, water pollution is a problem which has negative influence on aquatic ecosystem and public health. Due to the persistent organic compounds in pesticides, it is on the rise. The migration of pesticide residues to water influenced by certain parameters including rainfall, drainage, microbiological activity, soil temperature, mobility and partial solubility of pesticide in water etc. The extensive utilization of pesticides for enhancing agricultural growth rigorously affected the surrounding ecosystem and contaminated water has been an area of apprehension. Metal-organic frameworks (MOFs), new type of porous materials, made up of two basic components: organic linkers and clusters of metal ions. They are well-known for their outstanding features and efficient applications. MOFs are regarded as the promising contenders for pollutant eradication and adsorption due to its uniformity in size, tuneable pore size and high surface area etc. In the present study, Zn-supported bimetallic metal-organic framework has been synthesized by hydrothermal method successfully.The synthesized Zn-BiMOFs material was characterized by UV-Vis, FT-IR, Powder-XRD, FE-SEM and EDAX studies. The adsorption property of the synthesized MOFs has investigated by agricultural real time pesticide like pendimethalin as a sample pollutant. From the characterization studies, the wavelength and band gap values of the Zn-BiMOFs were found to be 239 nm and 2.7 eV respectively. The functional groups present in the bimetallic metal-organic frameworks were confirmed by FT-IR analysis. The obtained FT-IR peaks at 632 and 537 cm^{-1} revealed the presence of metal-oxygen bond successfully. The crystallite size and phase of the MOFs were found to be 10.9 nm and monoclinic structure confirmed by XRD analysis and there was rod-like morphology found by FESEM analysis. The adsorption study was carried out by changing three different catalyst weights such as 5, 7.5 and 10mg and concentration of the pesticide solution maintained to be 30 ppm with neutral pH. During the adsorption study, the percentage (%) efficiency of the prepared Zn-BiMOFs catalyst was calculated to be 86, 93 and 96 % respectively. In addition to that pseudo-second-order kinetic model was done and demonstrated that pendimethalin chemisorption occurs effectively on the surface of synthesized Zn-BiMOFs materials. As a result, it is concluded that the synthesized Zn-BiMOFs exhibit high potential for the removal of pesticides.

Keywords: BiMOFs; Pesticide; Morphology; Adsorption; Analysis, Parameter.

1. Roy, D., Neogi, S., & De, S. (2021). Adsorptive removal of heavy metals from battery industry effluent using MOF incorporated polymeric beads: A combined experimental and modeling approach. *Journal of Hazardous Materials, 403*, 123624.

OP-35

POLYDOPAMINE COATED HYBRID MEMBRANES BASED ON POLY (AMIDE IMIDE) AND UIO-66 WITH IMPROVED PERMEATION AND ANTIFOULING CHARACTERISTICS

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Abstract

In this study, zirconium-based metal-organic framework (Zr-MOF), named UiO-66 was synthesized by solvothermal method and coated by polydopamine (PD) to obtain PAI/UiO-66/PD membranes. The bare PAI and PAI/UiO-66 membranes were prepared and immersed in PD to fabricate PAI/PD and PAI/UiO-66/PD membranes. The PD coated membranes were showed enhancement in pure water flux (PWF), water uptake, porosity, hydrophilicity, BSA and HA rejection and flux recovery ratio. The FT-IR was employed to probe the chemical functionalities of the membranes. The top surface and cross-section SEM images were evidenced that the coating of PD is significantly altered the membrane morphology. The water uptake and porosity of the membranes were also measured to evaluate the enhancement in hydrophilicity of PAI/UiO-66/PD hybrid membranes. The antifouling capacity of the PAI/UiO-66/PD hybrid membranes was evaluated using BSA and HA fouling agents and found that higher flux recovery ratio of 94.8% and 79.2% for the filtration of BSA and HA solutions respectively. The PAI/UiO-66/PD membrane was also exhibited the highest

rejections of 93.5% and 92.5% for BSA and HA solutions. Overall results demonstrated that the superior permeation, separation and antifouling behaviour of PAI/UiO-66/PD membrane and thus promising for possible use as UF membrane in water and waste water treatment.

OP-36

Custom-made proton exchange membranes based on chitosan and sulfonated octaphenyl polyhedral oligomeric silsesquioxane (S-POSS) FOR DMFC applications

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Abstract

Direct methanol fuel cells (DMFCs) have emerged as a promising clean energy device due to their high energy density and environmental advantages. In this study, a novel approach to enhance the performance of chitosan-based PEMs by incorporating sulfonated octaphenyl polyhedral oligomeric silsesquioxane (S-POSS) nanoparticles is presented. Direct methanol fuel cells (DMFCs) have emerged as a promising clean energy device due to their high energy density and environmental advantages. In this study, a novelThe chemical functionality of S-POSS is verified by Fourier transform infrared (FTIR) and X-ray diffraction (XRD) spectroscopic studies. The surface morphology and roughness of Chitosan/S-POSS membranes were explored in terms of scanning electron microscopy (SEM) and atomic force microscopy (AFM) whereas the distribution of S-POSS nanoparticles and proton conductivity were probed by energy dispersive X-ray (EDX) analysis and AC impedance spectra. Physico-chemical characteristics such as ion-exchange capacity (IEC), water uptake and oxidation stability were found to be increases after the addition of S-POSS into Chitosan matrix. Increment in S-POSS

content in Chitosan matrix decreases the surface contact angle due to the increase in hydrophilicity. Further, the dispersing ability S-POSS in Chitosan matrix is evidently shown by an increase in surface roughness of the Chitosan/S-POSS nanocomposite membranes. On the whole, Chitosan/S-POSS membrane showed the highest proton conductivity of 5.59×10^{-3} Scm^{-1}, selectivity of 7.9×10^{4} $Scm^{-3}s$ and lesser methanol permeability of $3.52\times10^{-8}cm^{2}s^{-1}$. The strong interfacial interaction between Chitosan and S-POSS in nanocomposite membranes create strong hydrogen bond network to facilitate the proton conduction pathway *via* both vehicle and Grotthuss type mechanisms. Overall results suggested that the Chitosan/S-POSS nanocomposite membranes were superior and appropriate alternative for commercially high-cost Nafion® membranes for use in renewable direct methanol fuel cell (DMFC) devices.

OP-37

NOVEL SOL-GEL SYNTHESIZED MULTI-ACTIVE GRAPHENE OXIDE-AEROGEL (3D) FOR REDUCTION OF NITROPHENOL COMPOUND

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Abstract

Industrial revolution happened in 18th century created major threat for environment especially for water resources. Large amount of toxic chemical compounds like phenols in water directly led to nausea, fatigue etc. Because of the photochemical reaction of higher aromatic compounds, certain organophosphate pesticides, insecticides the nitrophenols were formed and remained hotspot among other toxins. Furthermore, growing population is strongly pressing already existing crises for freshwater. To maintain sustainability there exist an immediate need for the formulation of new active compounds with improved efficiency. In this

work, we have formulated metal free graphene oxide-aerogel (3D) for the reductive elimination of nitrophenol compound effectively. graphene oxide-aerogel is considerably lighter solid with average pore size in the range of 1-50 nm in diameter respectively. Initially the graphene oxide was prepared using hummers method and formulated into aerogel (3D) structure using sol-gel technique. From the XRD analysis, a diffraction peak at 10 ° (2θ) confirms the formation of graphene oxide-aerogel. The Raman spectra included two prominent D and G bands at 1310.55 and 1591.08 cm^{-1} respectively which attributed to the vibration of sp^3 (C-C) and sp^2 (C=C) in graphene oxide-aerogel. Furthermore, λmax value of graphene oxide-aerogel was found to be at 230 nm corresponds to π-π^* transitions in C=C bond and a broad shoulder near 300 is due to the presence of n- π^* transitions of carbonyl groups. The FT-IR study confirmed the abundant functional groups on the GO edges/surfaces have given rise to the higher chemical reactivity and presence of C=O, C=C at 2341 and 1627 cm^{-1} respectively. Also there was the identification of sponge like morphology identified by FE-SEM analysis. The catalytic efficiency has investigated by the reduction of 4-nitrophenol using synthesized graphene oxide-aerogel (3D) by maintaining three different catalyst weights like 5, 7.5 and 10 mg respectively. The concentration of the nitrophenol source has maintained to be 0.25 mM solution at natural pH. During the study the catalyst exhibited complete reduction within 30, 22 and 12 minutes respectively. Hence the catalyst weight is indirectly proportional to the time for complete reduction. So, it is concluded from the result that the presence of highly active sites on the surface to speed-up the reaction by the holey 3D structure of the graphene oxide-aerogel.

OP-38

Light activation properties of Multiferroic $BiFeO_3$ nanostructures made using Ethylene glycol-based sol-gel strategy

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Abstract

Uniform BiFeO3 nanoparticles with a tightly controlled particle size distribution were achieved using a straightforward glycol-based sol-gel process at a low temperature of 100°C. Characterization techniques including X-ray diffraction (XRD), thermogravimetric analysis coupled with differential thermal analysis (DTA/TG), and transmission electron microscopy (TEM) were employed to analyze the synthesized powders. Rapid heating (calcination) followed by immediate cooling (quenching) to room temperature were identified as critical factors for the production of pure BiFeO3. Differential scanning calorimetry (DSC) analysis confirmed the transition to a ferroelectric state, solidifying the ferroelectric nature of the prepared BiFeO3 nanoparticles. The robust light absorption at 2.65 eV and the amplified photocatalytic activity observed with the addition of H_2O_2 suggest promising applications in wastewater treatment.

Keywords - Multiferroic $BiFeO_3$, Sol–gel, Photocatalytic Activity, DSC

OP-39

EFFECT OF PERCHLORATE ON FIREWORK COMPOSITION

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Abstract

Potassium Perchlorate ($KClO_4$) containing pyrotechnic mixtures is more sensitive to friction, electrical and impact. The pyrotechnic formulations containing $KClO_4$ (oxidizer) were studied for sensitivity (mechanical and electrical) study with different types of fuels. Sensitivity of pyrotechnic formulations contains $KClO_4$, Viton A, sulphur and graphite powder also studied. The impact sensitivity, friction sensitivity and electrostatic sensitivity are studied by Bureau of explosives impact machine (BOE Impact Test), BAM Friction Test Apparatus and Electrostatic Discharge Test Instrument (ESD testing) respectively.

Keywords: Potassium Perchlorate, BAM Friction, Impact Test, Electrostatic Discharge

OP-40

PALLADIUM (II) COMPLEXES WITH QUINOXALINE BASED SCHIFF BASE LIGANDS: SYNTHESIS, STRUCTURAL AND BIOLOGICAL STUDIES

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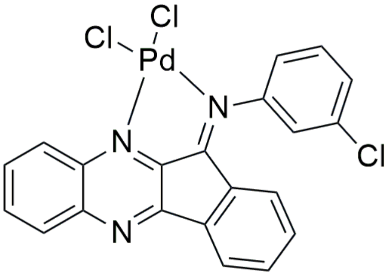
Abstract

Schiff base metal complexes play an important role in many applications such as biological, catalytic activity, and optical property. In this work, New quinoxaline based Schiff base ligand was derived from 1,2-diamineketone and aniline in presence of ethanol. $PdCl_2$ react

ligand to form typical compound $PdCl_2(L)$. Schiff base metal complexes were characterized by using FT-IR, NMR, Mass and UV–Visible spectral studies. The molecular structure of complexes was confirmed by single crystal X-ray diffraction method. Selected metal complexes were evaluated biological studies.



OP-41

BIOPOLYMER COATING ON AZ31B Mg ALLOY AS AN IMPLANT WITH ENHANCED DRUG DELIVERY AND ANTIMICROBIAL PROPERTIES

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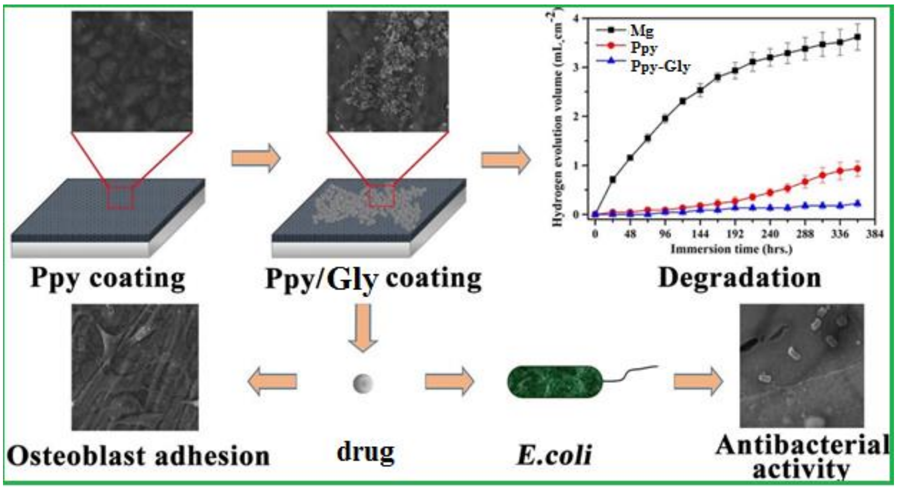
Abstract

Implant-related infection is one of the major concerns in orthopedic surgery. Typically, infection incidence ranges from 0.7% to 4.2%, following post-operative surgery. Failure of the orthopedic implant due to bacterial infections and poor osseointegration is a common problem in total hip arthroplasty. Conventional drug therapies have some limitations, such as very low drug solubility, lack of selectivity, poor distribution, serious side effects, unfavorable for pharmacokinetics, high dosage and are toxic to non-target tissues. Therefore, to solve these

obstacles, the local antibiotics of drugs are incorporated at the implantation site, which is an effective approach to reduce the implant associated infection. Electropolymerisation of biopolymer coatings on metallic implant surface, impregnated with antibiotic is found to be a solution. Hence, In the present study we have developed glycine-pyrrole biopolymer coating on anodized AZ31B Mg alloy by electropolymerisation. Then the coating was loaded with gentamicin drug by dip coating method. SEM and IR studies confirmed successful biopolymer (Glycine and Pyrrole) coating. Copolymers makes easy interaction with drug molecule gentamicin and it release drug slowly through electrodeposition coating method. This structure offered an improvement in gentamicin drug loading by 145% (16 µg/mm^2) and increased the drug release duration (in days) by almost 5 times than pyrrole alone coatings. The copolymer with drug delivery platforms demonstrated a prolonged drug release and in vitro inhibitory effect on the growth of the S. aureus. In addition, the bioactivity of the coatings was examined after the bio-mineralization process in the simulated body fluid. In conclusion, the developed Mg- poly(Py-co- Gly) – gentamicin drug coating system shows great potential for improving self-antibacterial performance, bioactivity, and longevity of Mg-based biomaterials.



OP-42

SYNTHESIS OF CARBON ELECTRODE MATERIAL FOR ENERGY STORAGE APPLICATION USING $FeCl_3$ ACTIVATED BIOMASS

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Abstract

Energy storage technologies with practical uses including batteries and supercapacitors. The poor performance of the electrode was impeded the development of these energy storage devices. Due to its low cost, ease of processing, and excellent stability, biomass from waste plants presents a promising green option for energy storage device electrodes. This work describes the research of using lotus seedpods (LS) as a biomass precursor in a two-step fabrication to convert biomass into activated carbon electrode material with high electrical conductivity. First, the LS is precarbonized and then subjected to simultaneous pyrolysis and activation with $FeCl_3$, resulting in LS-derived activated carbon material. The activated carbon material's structural and functional properties were analyzed using XRD, Raman, and FT-IR analyses. The morphology and texture of carbon materials were examined using SEM and BET analyses. Activated porous carbon prepared in this study showed a BET surface area of 99.614 m^2/g and an average pore size of 3.52 nm. Based on these results, the electrode produced from this carbon material is expected to be an excellent electrode material for energy storage applications.

Keywords: Lotus seedpod, $FeCl_3$, Pyrolysis process, Electrode material, Energy storage devices.

OP-43

GREEN SYNTHESIS AND CHARACTERIZATION OF IRON OXIDE NANOPARTICLES BY BLUE clitoria ternates LEAVES EXTRACTS

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Abstract

Recent advances in nanoscience and nanotechnology have also led to the development of novel nanomaterials, which eventually raises the risk to human health and the environment. Interest in developing the green synthesis of iron oxide nanoparticles using Blue Clitoria Ternatea leaves extract. Investigations with x-ray difraction, Fourier-transform infrared spectroscopy, scanning electron microscopy and ultra violet spectroscopy were performed to know and understand more about the chemical structure and surface morphology of the synthesized iron oxide nanoparticles. The synthesized nanoparticles are formed by agglomeration of spherical and mono-disperse grains. XRD analysis reveals that the grains are polycrystalline with an average crystallite size of 20 nm. The FT-IR spectroscopy confirms the presence of the peak located at 592 cm^{-1} is assigned to stretching vibration of the Fe–O bond. UV-vis spectrum of synthesized Fe_3O_4 nanoparticles shows the characteristic surface plasmon absorption band is observed at 405 nm for the Fe_3O_4 nanoparticles synthesized by greener method.

Keywords: Nanoparticles, Blue Clitoria Ternatea, Greener method & Magnetite

OP-44

STRATEGICAL DESIGN AND SYNTHESIS OF DONOR-ACCEPTOR-BASED PHENANTHRO[9,10-D]IMIDAZOLES FOR IMPROVED *worm* MEMORY PERFORMANCE

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Abstract

Donor-acceptor systems are crucial in advancing organic resistive memory devices, offering tailored electronic properties that enhance performance and functionality in emerging memory technologies. We have designed and synthesized donor-acceptor (D-A) based compounds for non-volatile memory device applications. The imidazole core was substituted with carbazole, fluorene, dibenzothiophene, and dibenzofuran unit to get a binary Write Once Read Many (WORM) memory. The optical investigations revealed an absorption maximum of 390 nm in fluorene-substituted imidazole, which confirms the intramolecular charge transfer from the donor to the acceptor unit. Besides, the electrochemical study exhibited an irreversible anodic peak in the range of 0.99-1.21 V, with a bandgap of 3.19-3.25 eV. The well-connected network in the film facilitates the charge transport between the donor and acceptor units. All the fabricated devices exhibited the non-volatile binary WORM memory characteristics. The compound substituted with fluorene in the imidazole core showed a maximum current ON/OFF ratio of 10^6 with a low threshold voltage of -0.99 V. Notably, the compound with carbazole attached to imidazole moiety displayed the ON/OFF current ratio of 10^5 with the low threshold voltage of -1.32 V. The stability of the devices was measured with retention and endurance

characteristics up to $4x10^3$ s and 100 cycles. The molecular simulations unveiled the plausible mechanism for binary memory with charge transfer and charge trapping. The charge traps in the molecular backbone confirm the electron-withdrawing nature of the imidazole unit. These studies would provide valuable insights for developing effective donor-acceptor molecular systems and improving the efficiency of resistive memory devices.

OP-45

ONE-POT SYNTHESIS OF HIGHLY FLUORESCENT CARBON DOTS FOR THE SELECTIVE DETECTION OF 6-MERCAPTOPURINE ANTICANCER DRUG

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Abstract

The cancer is the second biggest cause of death, with cardiovascular diseases being the only other main cause of death. Chemotherapy is primarily employed in cancer treatment due to the rapid growth and multiplication of cancer cells compared to most cells in the body. 6-mercaptopurine (6-MP) is a medication used in the treatment of certain types of cancer, particularly acute lymphoblastic leukemia, as well as certain autoimmune disorders like Crohn's disease and ulcerative colitis. Excessive use of 6-MP can cause liver damage, including hepatitis and liver failure.

In modern years, fluorescence based sensor has been very much attraction due to its high sensitivity, less time consumption and cheap cost. In particularly, carbon dots have a high aqueous stability and photostability, cheap cost, high fluorescence, easy surface

functionalization, excitation dependent and minimum toxicity. Carbon dots have shown excellent potential for sensing various analytes, including ions, small molecules, biomolecules and gases. Their sensitivity, selectivity and rapid response make them valuable tools for environmental monitoring, medical diagnostics, food safety and homeland security applications.

Keeping these objectives in our mind we have developed the fluorescence sensor of 6-MP by using dibenzoyl-l-tartaric acid capped carbon dots (DCDs). The synthesized carbon dots for stable for more than 4 months. Further, we have characterized by the fluorescence, UV-Vis, XRD, Raman and HR-TEM techniques. Interestingly, after the addition of 6-MP drug in the DCDs the fluorescence was quenched. We have calculated the limit of detection (LOD) to be 33.6 nM . Importantly, dibenzoyl-l-tartaric acid capped carbon dots (DCDs) was high selectivity compared with the higher concentrations of other co-existing biomolecules. Finally, we have applied the system for the sensing of 6-MP in blood serum and urine sample.

OP-46

MULTIFUNCTIONAL NANOFILLERS FABRICATION OF BIOCOMPOSITE FILMS: ENHANCING MECHANICAL PROPERTIES FOR BIOLOGICAL STUDIES

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Abstract

In this study to developed the biocomposite film from crustacean waste products used for biological applications. Combining polymers/nanofillers imparts specific functionalities of biopolymers and enhances its thermomechanical, biocompatibility and biodegradability properties. In this context, different combination of chitosan (Cs), synthetic polymer poly vinyl alcohol (PVA), nanofillers of bentonite clay (BC) and silver nanoparticles (Ag) biocomposite films prepared by casting method. The surface of the BC possesses the ability to attract and bind silver ions, thereby encouraging their transformation into silver nanoparticles through reduction, the average crystalline size 22nm. Physicochemical analyses results confirmed CS/PVA/BC/Ag composite film exhibits strong electrostatic interaction exhibit the better uniform dispersion with the polymer matrix to improve thermal stability and tensile strength. Swelling ability of composite film improve the hydrophilicity with a contact angle of 79.40° to control the releasing of AgNPs and polymer matrix diffusion. Biocompatibility and in-vitro anti-skin cancer activity tested using MTT assay method showed the film demonstrates effective adhesion to cancer cell membranes, inhibiting cell growth (90%) leading to cell apoptosis. AOEB and DAPI image attributed the nuclei changes for cell apoptosis. These findings highlight its potential in cancer treatment particularly for skin cancer .

Keywords: Chitosan, Biocomposite film, Biodegradable, Release kinetics, *In-vitro* studies.

OP-47

DEFECT ENGINEERING INDUCED ELECTRONIC REDISTRIBUTED BIMETALLIC LAYERED DOUBLE HYDROXIDE NANOSHEETS FOR HIGH ENERGY SUPERCAPACITOR APPLICATION

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Abstract

Modifying and upholding the surface-active site is a crucial approach for improving the performance of supercapacitors. In the present study, the mismatched integration of Ni in MnV-LDH matrix (Ni-MnV LDH) with surface defects have been developed, which assists for improved charge carrier transport properties. This work effectively demonstrates the tailored formation of cation vacancies in MnV LDHs nanosheets. The as-synthesized different molar ratio Ni^{2+} ions intercalated MnV LDH indexed as monoclinic structure with space group: C2/m, the SEM results illustrate the nanoflowers formation, caused by the accumulation of nanosheets, particularly the $Ni_{0.25}$-$Mn_{0.75}$V-LDH electrode exhibited larger area from CV curve and longer charge-discharge time compared to the other molar ratios Ni-MnV LDH/NF electrodes. This electrode manifested high specific capacitance of 3504 F g^{-1} at 1 A g^{-1} Current density and lower charge transfer resistance (R_{Ct}) of 0.4 Ω. Furthermore, the Ni doped bimetallic layered double hydroxides exhibit a overall enhanced electrode activity when compared to both bare MnV-LDH and other related reported electrode materials. Therefore, the present defect engineering process may provide an economical and fiscally feasible means of investigating high-performance electrode materials for high energy supercapacitor application.

OP-48

SYNERGISTIC EFFECT OF TMDCS/ g-C_3N_4 NANOCOMPOSITES MATERIALS FOR SUPERCAPACITOR APPLICATION

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Abstract

Supercapacitor (SC) devices holds an important position between traditional capacitors and metal - ion batteries in terms of energy density and power density values. In particular, SC's have greater power density values than Li-ion batteries make them useful for some specific applications, such as storing energy in hybrid cars. Increasing energy density values is one of the key challenges for the SC community. Transition metal dichalcogenides (TMDCs), are one of the new developing important material systems to have this potential, compared to their counterparts' transition metal oxides and conductive polymers. Here in this work, we proposed a MnS_2 and MnS_2/g-C_3N_4 nanocomposite for the energy storage application, exhibit the synergistic interactions between individual MnS_2 and g-C_3N_4. It emphasizes the interaction of both the elements within a system with enhance electrochemical performance, as well as cyclic stability of the electrode. The hybrid composite electrode materials shows superior specific capacity (Cs) of 1134.25 C g^{-1} at 1 A g^{-1} in 2 M KOH aqueous electrolyte, which is comparatively higher than that of pure MnS_2 spheres (814.13 C g^{-1} at 1 A g^{-1}). The assembled MnS_2/g-C_3N_4//AC Hybrid device (HD) exhibited a maximum specific capacity of 191.8 C g^{-1} at 1 A g^{-1}, which is potential candidate for commercial applications.

Keywords: Supercapacitor, Transition metal dichalcogenides, Graphitic Carbon Nitride.

OP-49

HIGH ENANTIOSELECTIVE SYNTHESIS OF CYANOPYRROLIDINE DERIVATIVES

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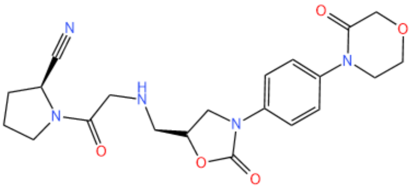
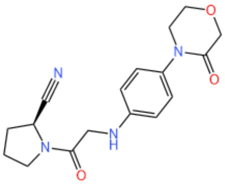
Abstract

In the search for potent and selective inhibitors of dipeptidyl peptidase IV (DPP-IV), we synthesized a series of 2-cyanopyrrolidine derivatives featuring a constrained imidazolidin ring and assessed their efficacy against DPP-IV. The majority of these compounds demonstrated submicromolar inhibitory activities against DPP-IV. Our work includes a novel process for the preparation of (S)-1-((((R)-2-oxo-3-(4-(3-oxomorpholino)phenyl)oxazolidin-5-yl)methyl)glycyl)pyrrolidine-2-carbonitrile (I) with exceptional chemical and enantiomeric purity, along with compositions containing this compound. Additionally, we present (S)-1-((4-(2-oxomorpholino)phenyl)glycyl)pyrrolidine-2-carbonitrile (II), along with the corresponding preparation processes and compositions. Furthermore, our work encompasses processes for determining the purity of these compounds, employing formula (I) and formula (II).



Formula (I)



Formula (II)

OP-50

DEVELOPMENT OF FLUORESCENT POLYETHENE CLADDING MATERIALS FOR PROTECTED CULTIVATION.

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Abstract

The growing of crops in environmentally controlled conditions is referred to as

protected cultivation or Greenhouse cultivation. Protected cultivation is a specialised production technology for high-value crops such as vegetables and cut flowers. In open-field cultivation, crops are grown at specific seasons to suit their growth, whereas this greenhouse production technology helps to overcome the seasonal barrier, ensuring year-round crop production. This benefits the farmers to produce crops even during the off-season (season not suitable for growing specific crops), fetching higher profitability. Generally, protected cultivation enhances crop duration, crop yields, and net profits compared to open field conditions. Low-cost and readily available polyethene (PE) monolayer films are commonly used as cladding materials, which last 2-3 years and have thicknesses of 140-200 μm. Light diffusion in greenhouse cladding materials is critical for crop growth and development. Light quality in terms of wavelength decides the current photosynthesis in crops. Generally, crop photosynthesis occurs only in blue (400–500 nm) and red regions (600–700 nm) of light, which are called photosynthetically active radiation and account for less than 15 per cent of total solar radiation. In theory, if the currently unused regions outside photosynthesis active radiation are made available for crop’s photosynthesis under greenhouse conditions, then the overall productivity will be improved in crops. The up-conversion of UV radiation can help reduce crop pest infestations in greenhouse conditions. Otherwise, UV radiation encourages the host identification and feeding behaviour of insects. There is experimental evidence to demonstrate the yield increase of 15-20 per cent under spectral conversion technologies in greenhouse conditions. Spectral conversion materials such as organic and inorganic dyes, phosphors and quantum dots are promising candidates to use as additives in poly-films to convert the wavelength of the unused spectrum of light for photosynthesis into either blue or red regions. This down or upconversion of light will facilitate the availability of more light for higher photosynthesis and crop yields.

OP-51

SYNTHESIS OF ZINC-DOPED SILICA XEROGEL AND ELECTRO-SPUN FIBER FOR ANTIBACTERIAL APPLICATIONS

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Abstract

We present ex-situ synthesis of zinc-doped silica Xerogel and electro-spun fiber at three distinct concentrations (low, medium, and high). While increasing the concentrations of silica, the gelation period was decreased (low, medium, high): 45 minutes, 30 minutes, and 15 minutes at 30°C ambient temperature and pressure conditions. The collected Xerogel powder was used to create electro-spun fibers with a diameter of around 60 nm-275 nm. The formation of Zinc doped silica Xerogel and electro-spun fiber was confirmed by Fourier Transform Infrared Spectroscopy and X-ray Diffraction studies, respectively. Both the Zinc doped silica Xerogels and the electro-spun fibers were found to exert excellent antibacterial properties against both '*Staphylococcus Aureus*' (gram-positive) and '*Escherichia Coli'* (gram-negative) bacteria through the Zone of inhibition method. There are prepared samples to utilize the MG63 cell line in the biomedical industry.

Keywords: Silica; Zinc; Xerogel; Biomedical; Polyacrylonitrile; Electro-spun Fiber.

OP-52

REAL APPLICATIONS OF SUPERCAPACITOR WITH CO_3O_4-CARBON QUANTUM DOT NANOCOMPOSITE BY ELECTROCHEMICAL PERFORMANCE

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Abstract

Carbon materials like graphene, carbon nanotubes and quantum dot doped with metal oxides have much more attraction in energy storage applications due to their sufficient surface area and efficient electrochemical activity. In the present work, carbon quantum dot (CQD) doped cobalt oxide (Co_3O_4) composite (Co_3O_4-CQD) is prepared using this cobalt nitrate and ascorbic acid (carbon source) through a facile hydrothermal method. The composite material functional groups, composition, surface area and surface morphology are evaluated by UV, FT-IR, XRD, Raman, XPS, BET, SEM, and TEM analysis. The electrochemical performance has been studied using the three-electrode system, the Co_3O_4 -CQD delivers the capacitance at 1209 F g^{-1} at 1 A g^{-1} and the capacitance remained stable after 3000 charge-discharge cycles. The asymmetric supercapacitor constructed using Co_3O_4-CQD and activated carbon (AC) (Co_3O_4-CQD//AC) as the positive as well as negative electrodes, respectively, which provided 13.88 wh Kg^{-1} energy and 684.65 w Kg^{-1} power density with 100% capacitance retention. The above results support that the Co_3O_4-CQD is a suitable electrode material for commercial supercapacitor applications.

Keywords: Carbon quantum dot; nanocomposite; Hydrothermal method; electrochemical performances; Supercapacitor.

OP-53

AN ULTRA-SENSITIVE DETECTION OF MELAMINE IN MILK USING RARE-EARTH DOPED GRAPHENE QUANTUM DOTS- SYNTHESIS AND OPTICAL SPECTROSCOPIC APPROACH

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Abstract:

The current investigation focuses on a rapid and sensitive spectroscopic approach to detecting melamine in food products using rare-earth Terbium doped Graphene Quantum Dots (Tb-GQDs) synthesized using simple chemical conjugation of Terbium and GQDs. Citric acid and diethylene triamine (DETA) are utilized as precursors in the synthesis of GQD. The synthesized Tb-GQDs were characterized using a variety of spectroscopic and microscopic techniques. Terbium, a rare earth element with exceptional fluorescence capabilities, is doped onto the surface of the GQD to achieve dual photoemission and photostability. The as-synthesized Tb-doped GQDs have a quantum yield of approximately 52%. Furthermore, Tb-doped GQDs function as a fluorescence probe, detecting and quantifying the melamine used as an adulterant in milk and milk products. Melamine was evaluated within a linear range of 0-5 µM and obtained a maximum detection limit of 0.31 µM. The proposed approach determined melamine in milk samples with an efficient recovery rate.

OP-54

DEVELOPMENT AND INVESTIGATION OF DOXORUBICIN CONJUGATED FLUORESCENT HYBRID CARBON DOTS FOR THE DRUG DELIVERY OF COLON CANCER.

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Abstract:

Cancer is one among the deadliest diseases in the world that affects the human health, and causes various implications to the growth metabolism. Herein, we focussed on the synthesis of Fluorescent Carbon Dots (CDs) based nanocarrier system for the effective detection and theranostics applications. In brief, rare earth Terbium doped CDs were synthesized using microwave method and characterized using various spectroscopic and microscopic methods. The difference in concentration of chemotherapeutic drug Doxorubicin (DOX) were interacted with the as synthesized nanomaterials and confirm their binding efficacy and drug release coefficient using various physicochemical methods viz. UV- Visible spectroscopy, Photoluminescence spectroscopy, Raman fluorescence spectroscopy, High Resolution Transmission electron microscopy (HR- TEM) and X-Ray Diffraction (XRD) respectively. The size and shape of the nanomaterials with and without drug moieties were confirmed using HR-TEM and found that the particles are biocompatible in nature with sizes ranges from 10-20 nm. The invitro activity of both Doxorubicin (DOX) and CD-Tb nanomaterials conjugated with drug molecules were studied against the Colon cancer cell line Caco2, the high cytotoxicity and changes in the morphology at tumour sites were observed by treating it with CD-Tb-DOX molecules. Thus, the invitro cellular cytotoxicity studies recommend the synthesized CD-Tb-DOX nanocarrier could appreciably improve in the metabolic damage of Colon cancer cell lines and benefits in the cell Apoptosis process.

Keywords: Fluorescent Carbon dots, Terbium Doxorubicin, anticancer drug, Colon Cancer, Nano carriers.

OP-55

DESIGN, STRUCTURAL ELUCIDATION, SPECTRAL CHARACTERIZATION AND BREAST CANCER DOCKING APPROACH OF 4-(tert-butyl)-2,6-bis (4-methoxy benzylidene)cyclohexanones

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Abstract

A cyclohexanone derivative of 4-(tert-butyl)-2,6-bis(4-methoxybenzylidene) cyclohexanone were synthesized by Claisen-Schmit condensation and the resultant were characterised by FT-IR, NMR and Single Crystal X-Ray diffraction analysis. Furthermore, some theoretical studies like Hirshfeld analysis and docking studies were carried out. Hirshfeld surface analysis of the compound was conducted in order to investigate the structure and its molecular properties like d_i, d_{norm}, 2D fingerprint plots and energy framework were done. Molecular docking studies of the title compound were carried out against breast cancer protein (3ERT) using Auto dock 4 Software. Results show that the compound can be a optimal candidate for treating breast cancer and be used as a pharmaceutical compound after necessary in vivo experimental studies.

Key words: Auto-Dock, breast cancer, Claisen-Schmit condensation, Hirshfeld analysis and Single crystal X-ray diffraction.

OP-56

Synthesis of Activated carbon supported on copper doped TiO_2 nanocomposite for photocatalytic activity studies

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Abstract

This study confidently explores the synthesis of TiO_2 nanoparticles, Copper -doped TiO_2, and Activated Carbon (AC)-Copper doped TiO_2 nanocomposites through a co-precipitation method. The nanocomposites of structural, optical, and morphological analyses was carried out. XRD analysis revealed that the TiO_2 nanoparticles had a tetragonal phase. FT-IR findings demonstrated functional groups of the nanocomposites. FE-SEM image of TiO_2, Copper doped -TiO_2 and AC- Copper-doped TiO_2 nanocomposite showed spherical shapes with aggregated and randomly distributed particles with an average size of 20-70 nm. The band gap energies of TiO_2, Copper-doped TiO_2 and AC-Copper-doped TiO_2 are found to be 3.14, 2.53, and 2.24 eV. Photoluminescence results show that the doping of AC and Copper have played an efficient role to inhibit the recombination of electrons holes pairs in TiO_2 during photocatalysis. Moreover, visible-light driven photocatalytic efficiency of the samples evaluated using Crystal violet dye as model contaminant. It was observed that AC-Copper doped-TiO_2 photocatalyst exhibited the higher degradation rate constant compared to the pure TiO_2. This excellent photocatalytic activity of AC-Cu-TiO_2 sample could be attributed to the morphology. The photodegradation response of Methylene blue dye under ultraviolet light irradiation was tested for the bare TiO_2, Cu-doped TiO_2, and AC-Cu-doped TiO_2 nanocomposites. Application study of photocatalytic studies.

Keywords: Nanocomposite, Photocatalysis, Cry

OP-57

Valorization of *Evolvulus alsinoides* Green Waste to Cellulose Nanocrystals via Sulphuric Acid Hydrolysis

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Abstract

As the world's population exponentially grows, so does the need for the production of food, with production growing annually from an estimated 1.0 billion to 2.5 billion tons within the last few decades. This rapid growth in food production results in an ever-increasing amount of agricultural wastes, of which already occupies nearly 50% of the total landfill area. For example, are the billions of dry tons of cellulose-containing plants disposed in landfills annually. This paper seeks to provide a method for isolating cellulose nanocrystals (CNCs) from *Evolvulus alsinoides*, in order to recycle and utilize the cellulosic waste material which would otherwise have no applications. CNCs have already been shown to have vast applications in the polymer engineering field, mainly utilized for their high strength to weight ratio for reinforcement of polymer-based nano composites. A successful method of purification and hydrolysis of *Evolvulus alsinoides* leaves was established in order to isolate usable CNCs. The CNCs were then characterized using current techniques to determine important chemical and physical properties. Fourier transform-infrared spectroscopy confirmed that hemicellulose and lignin were removed during the chemical pretreatments and hydrolysis. The HR TEM revealed a special characteristic spherical shape of the CNC. The findings of this study provide several avenues for valorization of green waste, while aiming to minimize the techno-economic impact of pretreatments and reduction of organic waste burning to reduce carbon in the atmosphere.

Key words: Surface modification, Agricultural waste, Cellulose nanocrystals, Acid hydrolysis, *Evolvulus alsinoides*

POSTER PRESENTATION

(PP)

PP-01

SYNTHESIS OF CARBON SUPPORTED ON CERIUM DOPED TIO$_2$ NANOCOMPOSITE USING *Azadirachta indica* LEAF EXTRACT AND THEIR CHARACTERIZATION, THERMAL, AND PHOTOCATALYTIC ACTIVITY STUDIES

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Abstract

This study confidently explores the production of TiO_2 nanoparticles, Cerium (Ce)-doped TiO_2, and Activated Carbon (AC)-Cerium doped TiO_2 nanocomposites through a green precipitation method. The products underwent thorough structural, optical, and morphological analyses. XRD analysis revealed that the TiO_2 nanoparticles had a hexagonal phase. FT-IR findings demonstrated the existence of certain chemical linkages. FE-SEM image of TiO_2, Ce- TiO_2 and AC- Ce-doped TiO_2 nanocomposite showed spherical shapes with aggregated and randomly distributed particles with an average size of 30-90 nm. The band gap energies of TiO_2 Ce-doped TiO_2 and AC-Ce-doped TiO_2 are found to be 3.10, 2.27, and 1.90 eV, respectively, indicating the enhanced efficiency of the nanocomposites. Photoluminescence results show that the doping of AC and Ce have played an efficient role to inhibit the recombination of electrons holes pairs in TiO_2 during photocatalysis. Moreover, visible-light driven photocatalytic efficiency of the samples evaluated using Methylene blue dye as model contaminant. It was observed that AC-Ce- TiO_2 photocatalyst exhibited the higher degradation rate constant compared to the pure TiO_2. This excellent photocatalytic activity of AC-Ce- TiO_2 sample could be attributed to the Spherical morphology. The photodegradation response of Methylene blue dye under ultraviolet light irradiation was tested for the bare TiO_2, Ce-doped

TiO_2, and AC-Ce-doped TiO_2 catalysts. After 160 min irradiation was photodegradation ability of the bare TiO_2 Ce-doped TiO_2, and AC-Ce-doped TiO_2 catalysts increased to 64.36%, 77.76%, and 93.27%.

PP-02

GREEN SYNTHESIS OF SILVER/SILVER OXIDE COMPOSITE USING LEUCAS ASPERA PLANT LEAVES EXTRACT FOR ANTIBACTERIAL ACTIVITY

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Abstract

Silver/silver oxide composite nanoparticles were synthesized using *Leucas aspera* plant leaves extraction process at room temperature. The prepared composites was characterised by FT-IR, UV–Vis spectroscopy, XRD analysis and SEM. The prepared nanoparticles showed characteristic UV–Vis absorption peak at 426 nm. The FT-IR vibration peaks show the formation of Silver/silver oxide composite nanoparticles , where the vibration peak for Ag-O is deliberately present at 546cm^{-1}.The characteristic peaks obtained in the XRD spectrum confirmed the formation of cubic face-centered Silver/Silver oxide nanoparticles. SEM images of the biosynthesized Ag/Ag_2O composite NPs exhibited spherical shape with average diameter of 38 nm. The synthesized samples were tested against antibacterial activity of *Staphylococcus aureus* and *Escherichia coli* and it is also favourable with cytotoxicity effect with human osteosarcoma (MG-63) cells.

Keywords: Silver/silver oxide , *Leucas aspera, Nanoparticles,* Antibacteria activity, Cytotoxicity

PP-03

IMPROVING THE CORROSION RESISTANCE OF THE NI-W-CEO$_2$ BY ELECTRODEPOSITION

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Abstract

Electroplated hard chromium coating is widely used as a wear resistant coating to extend the life of mechanical components. Composite coating has been identified as suitable materials for replacement of chromium coating. However, the electroplating process generates hexavalents chromium ion is carcinogen. Nanocomposite coatings were obtained by electrodeposition of CeO_2 nano-particles with Ni-W on mild steel surface. The structure, surface morphology, composition and corrosion resistance properties of the nanocomposite deposits have been characterized by using various techniques. XRD studies revealed that (111) plane was predominant in the Ni-W alloy and also in Ni-W-CeO_2 composites. The patterns of the electrodeposits confirmed that it had only fcc frame work structure. Scanning electron microscopy reveals smaller grains and uniform distribution of the CeO_2 in the alloy matrix. Microhardness increased with CeO_2 addition in the alloy. The corrosion behavior of the Ni-W-CeO_2 composite coatings was investigated by potentiodynamic polarization and electrochemical impedance spectroscopy in 3.5wt% NaCl solution. Moreover the addition of CeO_2 nanoparticles could significantly enhance the wear resistance of the coatings. The pulse current composites coatings offer uniform surface high microhardness and enhanced corrosition resistance than direct current composite coatings.

Keywords: Pulse current, XRD, Surface morphology, Corrosion resistance.

PP-04

ADSORPTION OF LEAD (II) IONS FROM INDUSTRIAL EFFLUENT BY USE OF EGGSHELL

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Abstract

Heavy metals are major toxicants found in industrial effluent and have been known to contaminate the water resources. They include metals such as lead, cadmium, arsenic and chromium which pose a significant threat to the environment and public health because of their toxicity, accumulation along the food chain and their recalcitrance in nature. The aim of the study was to investigate the removal of lead (II) ions from raw industrial effluent using low cost sorbent; eggshell. Industrial effluent samples were collected through purposive sampling at the point of discharge before treatment. The lead concentration in the effluent samples collected was analyzed by use of the Atomic Absorption Spectrophotometer (AAS) (Spectra AA50). Crushed eggshell of different particle size were added to the sample stirred using magnetic stirrer for 30 minutes to attain equilibrium. After contact time, equilibrium uptake of lead (II) ions by the eggshell was achieved. Filter paper grade 54 was used to filter the eggshell so as to obtain the filtrate. The exact concentration of the filtrate was then determined using the AAS. This entailed the varying of process parameters like effects of pH, sorbent size, sorbent amount, and contact time in the sampled effluent. Results obtained were analyzed to compare the lead (II) ions removal efficiency between raw and boiled eggshells. Maximum adsorption of Pb^{2+} on eggshell was observed at pH = 5. Adsorption equilibrium was established in about

120 minutes and the mass of eggshell used was 10 g/L of particle size using sieve No. 355µm. Langmuir model was the best fitted model on the raw eggshell with a correlation coefficient $R^2 = 0.994$ and adsorption capacity of 11.63 mg/g, this was followed by Freundlich $R^2 = 0.926$ and then the Temkin Isotherm $R^2 = 0.875$. The results showed that the egg shell removed the lead (II) ions from the industrial effluent from 19.2 mg/L to 0.2023 mg/L which is below the recommended water quality standards for effluent discharge to public sewers within optimum conditions.

Key Words: Adsorption, Industrial Effluent, Lead (II) Ions Removal and Egg Shell

PP-05

ENHANCED ELECTROCHEMICAL PERFORMANCE OF $CuMoO_4$ NANOPARTICLES PREPARED VIA A LOW-COST HYDROTHERMAL METHOD

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Abstract

In this study, we synthesized $CuMoO_4$ nanoparticles using an economical hydrothermal method. These nanoparticles were characterized for their functional, surface, and electrochemical properties using FTIR, FESEM, and CV and GCD techniques, respectively. The FTIR spectra revealed a peak at 542.8 cm^{-1}, attributed to the MoO_3 lattice bending mode and the vibrational stretching of CuO_4. Microsphere-like structures with good porosity were observed in the $CuMoO_4$ during FESEM analysis. The CV curve at 10mV/s exhibits the faradaic redox behaviour of reactions. Furthermore, GCD exhibited a specific capacitance of 219 Fg^{-1} at 1 Ag^{-1}. These results suggest that $CuMoO_4$ nanoparticles demonstrate promising electrochemical performance.

Keywords: Hydrothermal method, $CuMoO_4$, specific capacitance, redox reaction, CV etc.

PP-06

BIO SYNTHESIS OF BIMETALLIC NANOPARTICALS AND THEIR ASSESSMENTS OF BIOLOGICAL ACTIVITIES

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Abstract

The green synthesis of nanoparticles using plant aqueous extracts is an ecofriendly and elegant technique. The present study focuses in the synthesis of ZnO / MgO nanoparticles using the leaves aqueous extracts of *Helictres isora*. This green synthesis approach shows that the environmentally benign and renewable aqueous extract of *Helictres isora* could be used as a reducing agent for the synthesis of bimetallic ZnO / MgO nanoparticles. The aim of this study is to synthesis and efficacy assessment of Zinc oxide / Magnesium oxide nanoparticles by anti-microbial, anti-cancer and antioxidant studies. The prepared ZnO / MgO nanoparticles were assessed under antimicrobial evaluations using two bacterial pathogens and two fungal pathogens. Anti-inflammatory analysis was carried out by using Bovine serum albumin each group has 5 samples or 10, 20, 30, 40, 50 microliter. Anticancer assessment was carried out by MTT Assay. Bimetallic nanoparticles synthesis shows the concentration exhibited promising results. At 100µl concentration, the zone of inhibition for all two spices Streptococcus mutans and Candida albicans, was <10 and for the anti-inflammatory activity for the bimetallic

nanoparticles were good results in higher concentrations showed acceptable within limits. Within the limits of the study, could be the Zinc oxide / magnesium oxide nanoparticles have remarkable antibacterial capabilities perhaps in nanomaterials to enhance their properties.

PP-07

SYNTHESIS AND CHARACTERIZATION OF NANOCELLUOSE CRYSTALS USING *Turbiaria conoides* BIOMASS

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Abstract

The growth of nanocellulose has outstanding interest in the last few decades owing to its unique and potentially useful features. Novel nanocelluloses improve the strongly expanding field of sustainable materials and nanocomposites. CNCs and CNFs are two kinds of nanocelluloses (NCs), and they own various superior properties, such as large specific surface area, high tensile strength and stiffness, low density, and low thermal expansion coefficient. Different methods of nanocellulose like pretreatment method, mechanical process and chemical hydrolysis used for the synthesis of nanocellulose. The sulfuric acid hydrolysis was in different acid concentration with room temperature and various reaction times.Their application includes nanocellulose in transdermal drug delivery, Hydrogels, Aerogel Systems, nanocellulose in tablet formulations and nanocellulose in microparticulate Drug Delivery. Characterization of cellulose includes scanning electron microscopy, x-ray diffraction (XRD) analysis FT-IR of samples and thermo gravimetric analysis

Keywords: Cellulose Nanocrystal, *Turbinaria conoides*, Biomass, FT-IR, SEM and XRD.

PP-08

PHYTO-MEDIATED SYNTHESIS OF BIMETALLIC NANOMATERIALS AND THEIR ANTIBACTERIAL, ANTIOXIDANT AND ANTICANCER ACTIVITIES

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Abstract

The green hydrothermal synthesis of nanoparticles using brown sea weeds extracts is an ecofriendly and elegant technique. The present study focuses the synthesis of ZnO / BaO nanoparticles using the aqueous extracts of *Turbinaria conoides*. This green synthesis approach shows that the environmentally benign and renewable aqueous extract of *Turbinaria conoides* could be used as a reducing agent for the synthesis of bimetallic ZnO / BaO nanoparticles. The aim of this study is to synthesis and efficacy assessment of Zinc oxide / Barium oxide nanoparticles by anti-microbial, anti-cancer and antioxidant studies. The prepared ZnO / BaO nanoparticles were assessed under antimicrobial evaluations using two bacterial pathogens and two fungal pathogens. Anti-inflammatory analysis was carried out by using Bovine serum albumin each group has 5 samples or 10, 20, 30, 40, 50 microliter. Anticancer assessment was carried out by MTT Assay. Bimetallic nanoparticles synthesis shows the concentration exhibited promising results. At 100μl concentration, the zone of inhibition for all two spices Streptococcus mutants and Candida albicans, was <10 and for the anti-inflammatory activity for the bimetallic nanoparticles were good results in higher concentrations showed acceptable within limits. Within the limits of the study, could be the Zinc oxide / Barium oxide nanoparticles have remarkable antibacterial capabilities perhaps in suture materials to enhance their properties.

PP-09

GREEN SYNTHESIS OF CHITOSAN/CUO COMPOSITE EMPLOYING *Hymenocallis littoralis* LEAF EXTRACT AND EVALUATION OF ITS ANTIBACTERIAL BEHAVIOR

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Abstract

Recently, copper oxide nanoparticles (CuO NPs) have emerged as promising antibacterial agents due to its functional properties. Several research works are focusing on the green synthesis methods and incorporation of CuO NPs with chitosan resulting in enhanced efficacy. The current study elucidates the synthesis, surface modification, and antibacterial activity of CuO NPs synthesised by utilizing the leaf extract of *Hymenocallis littoralis*. This method offers an eco-friendly alternative to other conventional methods, yielding nanoparticles with standard size and morphology. Also, the surface functionalization with chitosan further enhances the antibacterial property and bio-compatibility. The prepared composite was characterized using UV-Vis, FT-IR, XRD and TGA analysis. The morphological feature was investigated by HR-SEM analysis. CuO NPs show broad-spectrum activity against Gram-positive (*S. aureus*) and Gram-negative bacteria (*E. coli*) evaluated by means of agar well diffusion method. The antibacterial mechanism involves the membrane disruption, reactive oxygen species generation, and protein interaction, leading to bacterial cell death. Therefore, it is suitable for various biomedical applications including wound healing, implant coatings, and drug delivery systems in pharmaceutical sector.

Keywords: Chitosan, CuO Nps, Green synthesis, Antibacterial activity.

PP-10

SYNTHESIS OF Sn AND Ce BASED ZrO NANOCOMPOSITES AND ITS APPLICATION IN PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE DYE

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Abstract

To synthesis Sn and Ce based ZrO nanocomposites via., hydrothermal method. The synthesized ZrO_2, Sn/ZrO_4 and Ce_2/Zr_2O_7 were characterized by various analytical techniques such as XRD, FT-IR, SEM, and UV-DRS. The crystalline sizes of the synthesized ZrO_2, Sn/ZrO_4 and Ce_2/Zr_2O_7 were 27.8, 37.6 and 43.2nm, respectively. The morphologies of the prepared materials were investigated using SEM, it was discovered that ZrO_2, Sn/ZrO_4 and Ce_2/Zr_2O_7 nanocomposite showed rod, irregular and spherical shapes. UV-DRS analysis was used to determine the bandgap of the synthesized Sn/ZrO_4 and Ce_2/Zr_2O_7 which was found to be 2.0 eV, each. The prepared materials were used as a catalyst for the photodegrading of methylene blue dye among which Ce_2/Zr_2O_7 material showed high degradation of the dye molecules up to 90%.

PP-11

SYNTHESIS AND CHARACTERIZATION OF ZrO_2 NANOPARTICLES FOR SUPERCAPACITOR APPLICATION

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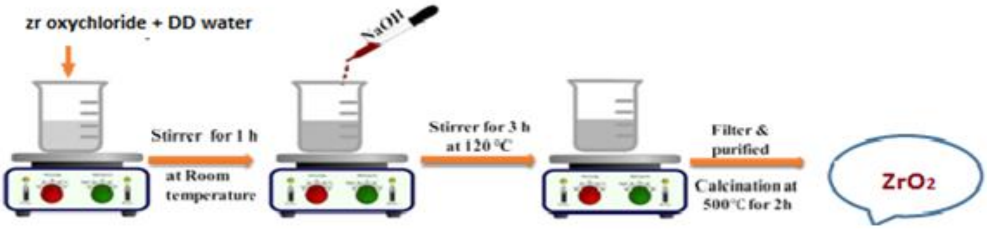
Abstract

The ultimate progress in population rate has made energy crisis all around the world which at the same time leads to high energy demand. Now, energy production and storage is major need along with the improvements in technologies. Electrochemical cells like batteries, supercapacitors and fuel cells serve as an excellent alternative eco-friendly energy sources that paved way for present generation of power production. Supercapacitors are found to have high power density, long life spanwith cyclic stability, etc… Electrochemical capacitors (ECs) based on transition metal oxides (TMOs) have been developed to a larger extent due to their ability to store huge energy via multiple redox states. In recent years, the ZrO_2 has been examined as a pseudocapacitive material for electrochemical supercapacitor applications. Synthesis methods like co-precipitation route, hydrothermal method, microwave-assisted technique and sonochemical method, etc., have been adopted to fabricate micro/nano architectures for metal oxides. Precipitation method is well suited for its merits. In present work, ZrO_2 nanoparticles have been prepared via co-precipitation route using NaOH as reducing agent. The structural, morphological and electrochemical features of the prepared materials were reported.

Keywords: ZrO2, Co-precipitation,nanopowder, Supercapacitor, electrochemical studies.



PP-12

BIO-FUNCTIONALIZED CHITOSAN COATED IRON OXIDE NANOCOMPOSITE: A DUAL ACTION STRATEGY FOR ATTENUATING BACTERIAL PROLIFERATION AND FREE RADICAL ELIMINATION

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Abstract

The formulation of environmentally friendly, biologically inspired iron oxide nanoparticles (NPs) has come under intense scrutiny due to their exploitation in the biomedical sector. The incorporation of metal oxide Nps in a biopolymer matrix leads to significant alterations in their structural and functional characteristics. In the present work, iron oxide NPs were incorporated with chitosan in order to generate the potent antimicrobial and antioxidant agents. Chitosan has gained significant attention owing to its distinctive properties, including low toxicity, biodegradability, biocompatibility, and antibacterial capabilities. The objective of the present investigation is to fabricate chitosan-embedded iron oxide nanocomposite employing *Cissus quadrangularis* plant extract. It serves as a reducing and capping agent, facilitating rapid and eco-friendly synthesis of iron oxide Nps. The physicochemical and structural features of the samples were characterized by UV-Vis, FT-IR, XRD, XPS, HR-SEM, BET and TGA analysis. The antibacterial efficacy was examined in the strains of *S. aureus* and

E. coli, it showed that increase in the concentration leads to drastic inhibition in the growth of the microorganisms. The determination of the free radical scavenging capacity of the samples was conducted using the DPPH assay. Likewise, the samples were confirmed to be blood compatible through the hemolysis evaluation. The findings suggested that the chitosan-iron oxide nanocomposite may be extensively employed as a viable material for biomedical implements.

Keywords: Nanocomposite, antimicrobial, antioxidant, hemolysisS

PP-13

TAILORING COBALT OXIDE EMBEDDED N, S-DUAL DOPED HOLLOW CARBON SPHERES AS A BIFUNCTIONAL ELECTROCATALYST FOR ORR AND OER APPLICATIONS

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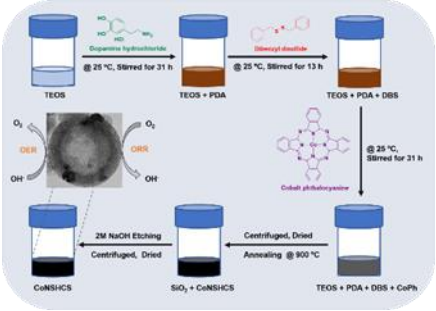
Abstract

Our ever-growing reliance on fossil fuels has fuelled a global warming crisis. Greenhouse gas emissions continue to rise, demanding immediate action. Metal-air batteries emerge as a compelling alternative, offering significant advantages over traditional lithium-ion batteries. They boast both lower costs and superior energy density. However, a key challenge lies in the rechargeable metal-air battery's cathode, where oxygen reduction (ORR) and evolution (OER) reactions occur during discharge and charge cycles, respectively. Both reactions suffer from high overpotentials due to the robust oxygen molecule. While platinum (Pt) and RuO_2/IrO_2 catalysts excel at ORR and OER, their high cost and scarcity limit their

widespread application. The development of cost-effective, bifunctional electrocatalysts that efficiently drive both ORR and OER is crucial for unlocking the full potential of metal-air batteries.Transition metals hold promise as catalysts for oxygen reduction (ORR) and evolution (OER) reactions in metal-air batteries. However, their inherently low electrical conductivity hinders performance. Carbon materials, with their high surface area, offer a solution by acting as a conductive support. In this work, we present cobalt oxide (Co_3O_4) decorated on N, S-dual heteroatom-doped carbon spheres as a bifunctional electrocatalyst for both ORR and OER. Co_3O_4 serves as the active center, boosting both ORR and OER activity. The N, S-doped carbon acts synergistically, providing crucial structural support while enhancing stability and electrical conductivity. The hard-template method, using tetraethyl orthosilicate (TEOS) as a silica precursor, was employed to achieve the desired sphere-like morphology. This method successfully yields Co_3O_4-decorated dual heteroatom-doped carbon materials that exhibit remarkable stability during both OER and ORR.



PP-14

FACILE FABRICATION OF CHITOSAN-ZNO USING *plectranthus amboinicus* EXTRACT WITH ENHANCED PHOTOCATALYTIC AND ANTIBACTERIAL ACTIVITY

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Abstract

In this study, the ecofriendly biosynthesis of chitosan-ZnO-*plectranthus amboinicus* (CS-ZnO-PLE) hybrid nanocomposite was synthesized by the simple precipitation method. The chemical bonding and crystalline behaviors of synthesized hybrid nanocomposites were confirmed by FT-IR and XRD analysis. The optical properties of hybrid nanocomposite were studied by UV-Vis DRS spectroscopy. The biopolymer connected ZnO NPs intercalated with PLE structure appeared in the nanometer range, which was confirmed by HR-SEM and TEM analysis. The thermal properties were studied using TGA analysis. The CS-ZnO-PLE hybrid nanocomposites have higher thermal stability than other composites. The photocatalytic activities of synthesized hybrid nanocomposites have been evaluated with two different dyes (methylene blue and drimarene red). The photocatalytic degradation of the CS-ZnO-PLE hybrid nanocomposite significantly improved its efficiency. Furthermore, the antibacterial activity was evaluated by the agar well diffusion method and tested against two strains of bacteria gram positive *(S.aureus)* and gram negative *(E.coli)* bacteria. It would be applied to the biomedical field.

Keywords: ZnO NPs, HR-SEM, TEM, Photocatalytic activity, Antibacterial activity.

PP-15

CHITOSAN-LOADED ZIRCONIUM OXIDE NANOPARTICLES AND ASSESSMENT OF ANTIBACTERIAL POTENTIAL

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Abstract

Metal oxide nanostructured materials are extremely fascinating areas of investigation due to their distinctive characteristics and practical applications in biomedical sectors. Currently, bio-polymer based ZrO_2 composites has received center of interest in the biomedical and pharmaceutical sectors due to its nontoxicity and biodegradability. The surface functionalization of chitosan enhances the biocompatibility and antibacterial potential. Herein, the composite is fabricated by green synthesis method employing *Ixora Coccinea* leaf extract as a reducing agent and chitosan as a capping agent. The physicochemical properties were characterized by UV-Vis, FT-IR, XRD, HR-SEM and TGA analysis. The prepared nanocomposite exhibits efficient antibacterial activity towards the Gram positive (*S.aureus*) and Gram negative (*E. coli*) bacterial pathogens, making them suitable for various biomedical applications, including wound healing, implant coatings, and drug delivery systems. This elucidates the potential of zirconia nanoparticles synthesized via green routes and integrated with chitosan as effective antibacterial agents for combating microbial infections.

Keywords: ZrO_2 NPS, Plant extract, Chitosan, Antibacterial.

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PP-16

ANATASE-RUTILE PHASE TRANSITION OF CA@TIO$_2$ NANOSTRUCTURES FOR THE REMOVAL OF ENVIRONMENTAL POLLUTANTS UNDER VISIBLE PHOTON ILLUMINATION

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Abstract

Regulating the crystalline structure of titanium dioxide is essential granting the potential purposes for oxide. In the present investigation, we employed X-ray diffraction to investigate the significance of calcium doping on the anatase-rutile transition of phase. Preparation of Calcium-doped TiO_2 by sonochemical approach, followed by sintering at 700 ^oC temperature encompasses a phase transition. The inclusion of calcium into the TiO_2 lattice was hampered by the calcium ion's greater radius when contrasted to the titanium ion. Ca@TiO_2 nanostructures exhibited a reduced estimated band gap energy compared to pristine TiO_2. The Ca^{2+} substitutes into the TiO_2 surface were demonstrated by the Fourier transform infrared (FT-IR) spectral investigation. By conducting photocatalytic decomposition of persisting Congo red (CR) dye during visible photon radiation exposure, the photocatalytic effectiveness of the produced Ca@TiO_2 nanostructures was examined. Ca@TiO_2 nanostructures have been discovered to have more catalytic capability than pristine TiO_2 nanoparticles. In 4 hours of exposure duration with the Ca@TiO_2 nanostructures, the maximal degradation of the CR dye, or 88%, was accomplished with efficient regeneration.

PP-17

SOLUBILIZES AND INTERACTION OF ANTIDIABETIC DRUG TENELIGLIPTIN IN ANIONIC, CATIONIC AND NONIONIC MICELLAR SURFACTANTS MEDIA: A EXPERIMENTAL STUDY

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Abstract

we have tried the solubilization of antidiabetic drug teneligliptin (TNG) in triple, i.e., anionic, cationic and nonionic surfactant media. The anionic surfactant used was ammonium dodecyl sulphate (ADS), cationic, cetylpyridinium bromide (CPB) and nonionic, pluronic F-127 (F-127). The characterizations employed were UV visible spectroscopy, conductivity and antioxidant studies. The interaction of the drug in ionic and nonionic surfactant mediums was compared. The results of the above experiments were compared with docking studies. The solubilization capacity of TNG in the three surfactant mediums was assessed and the best result obtained was with the pluronic F-127 (F-127) surfactant.

Key words: Surfactants, hydrophobic, antidiabetic, anti-oxidant, teneligliptin.

PP-18

SYNTHESIS AND SPECTRAL CHARACTERIZATION OF 2'-(4-FLUOROBENZOYL)-1'-(4-(METHYLTHIO)PHENYL)-1',2',5',6',7',7A'-HEXAHYDROSPIRO[INDOLINE-3,3'-PYRROLIZIN]-2-ONE: A COMPREHENSIVE EXPERIMENTAL, COMPUTATIONAL, DOCKING METHODS, SWISSADME, AND PROTOX-2.

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Abstract:

The synthesized compound 2'-(4-fluorobenzoyl)-1'-(4-(methylthio)phenyl)-1',2',5',6',7',7a'-hexahydrospiro[indoline-3,3'-pyrrolizin]-2-one, was derived from the Substituted Chalcone with synthesized substituted Isatin and L-proline in One-Pot Reaction. A Synthesized compound was approved by characterizations such as FTIR, ^{1}H, and ^{13}C NMR. The synthesized compound was compared with the experimental values to the computational values by utilizing 6-31G (d, p) as the basis set, Calculations have been made to determine the electrical dipole moment (μ) and initial hyperpolarizability (βo). The estimated outcome (βo) indicates that the chemical in the title may exhibit nonlinear optical (NLO) activity. Calculations were made of the molecular electrostatic potential (MEP) and the C, N, and H atomic charges. The HOMO-LUMO energies were determined, and natural bonding orbitals (NBO) were examined. Molecular docking studies against different Anti-malarial proteins proved that the synthesized compound exhibits better binding affinity. Furthermore, the compounds' physiochemical, toxicological, and pharmacokinetic properties were assessed using the SWissADME and Protox-2 web tools.

Keywords: Chalcone, Spiro-oxindole, Spectral Characterization, DFT, Molecular Docking, SWissADME, and Protox-2.

PP-19

PHOTOCATALYTIC ACTIVITY OF SYNTHESIZED Mn- DOPED NiO NPs USING NOVEL IPOMOEA STAPHYLINA LEAF EXTRACT

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Abstract

The present study synthesized NiO and Mn doped NiO nanoparticles using the simple, cost-effective co-precipitation approach, which involves Ipomoea staphylina leaf extract. The composition, shape, and other physiochemical properties of the synthesized nanoparticles were characterized using X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectroscopy, field emission scanning electron microscopy (FESEM) with energy dispersive X-ray (EDX), UV-DRS, and X-ray photoelectron spectroscopy (XPS). The average crystalline size of dopant (Mn) and bare (NiO) NPs is 12.56 nm and 22.82 nm, respectively. NiO and Mn doped NiO NPs with an optical band gap of 3.84 and 3.67 respectively, are used for a Kubelka-Munk function. In order to ascertain the oxidation states, XPS data is noted for Mn, Ni, and O. The photocatalytic results show that Mn-doped NiO NPs have a high capacity to remove Congo red (CR) dye when exposed to UV light. Nearly 93% of the CR dye was degraded, based on the results.

Keywords; Green synthesis, Ipomoea staphylina, Photocatalysis, NiO NPs, Mn doped NiO NPs.

PP-20

ELECTRODEPOSITED POLYANILINE AND SILVER ON LASER-SCRIBED INTERDIGITATED FLEXIBLE ELECTRODES FOR

WOUND pH SENSING

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Abstract

Considering the complexity of wound healing, it is crucial to have an impartial indicator to assess the progress of healing. The optimal criterion for such a measurement would be its ease of use, sensitivity, accuracy, repeatability, and elimination of patient discomfort. A pH of approximately 5.5 indicates healthy epidermis and wounds in the process of healing; conversely, an infected wound exhibits a pH range of 7–8.5, which is neutral or slightly basic, due to the presence of diverse bacteria and enzymes. In this work, a flexible pH sensor was fabricated with Polyaniline and Silver on Laser-Scribed interdigitated electrodes for effective wound management. PANI was electropolymerized on graphene through 30 successive cyclic voltammetric scans in the potential range from −0.1 to 1.2 V at 100 $mV.s^{-1}$. The Ag/AgCl pseudoreference electrode is formed on the graphene trace to finish the two-electrode cell. The obtained electrodes were tested as pH sensors in the range from pH 4 to 8, with an average sensitivity of -45 mV/pH, which is in close proximity to the Nernstian value, the sensor accurately monitors a pH range that is physiologically significant.

Keywords: wound healing, Polyaniline, pH sensor.

PP-21

BIOINSPIRED SYNTHESIS OF CHITOSAN / ZnO COMPOSITE WITH ENHANCED ANTIBACTERIAL ACTIVITY

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Abstract

Nanotechnology is an expanding area of research in present-day science and technology, because of its versatile range of applications. Primarily, metal oxide nanoparticles provide significant potential for diverse applications, especially in the biomedical industry. Currently, there has been a significant focus on the bio-inspired production of Zinc oxide nanoparticles (ZnO NPs) employing plant extracts. This method is gaining attention due to its environmentally benign nature, low cost, and easy synthesis process. In the present investigation, ZnO NPs were fabricated through *Calotropis gigantea* leaf extract and incorporated in the chitosan matrix. Chitosan (CS) is the most abundant naturally occurring polysaccharide that is both biocompatible and biodegradable polymer. The UV-Vis and FT-IR techniques were used to investigate the optical properties and characteristics of functional groups. The crystalline structure, thermal stability and morphological features were examined using XRD, TGA and HR-SEM analysis. Subsequently, the antibacterial efficacy of the synthesized nanocomposite is assessed against Gram-positive (*S.aureus*) and Gram-negative (*E. coli*) bacterial pathogens.

Keywords: Chitosan, ZnO Nps, Antibacterial activity.

PP-22

FIRST-PRINCIPLES STUDY OF COBALT SUBSTITUTED $LiMn_2O_4$ AS CATHODE OF Li ION BATTERY

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Abstract

The increasing demand for energy storage and transportation devices, such as plug-in hybrid electric vehicles, needs the development of advanced battery electrode materials with high energy density, power, thermal stability, longer life cycles, and improved performance. First principle density functional theory calculations play a crucial role in optimizing and developing electrode materials for these energy storage applications. According to the literature survey, $LiMn_2O_4$ (LMO) was identified as an efficient cathode material for Li-ion batteries (LIB), offering a similar to the commercialized $LiCoO_2$ cathode materials. However, despite its good thermal stability, LMO has been found to have a relatively shorter cycling stability. To enhance its stability, the substitution of cobalt was explored, leading to the formation of the $Li_2Mn_3CoO_8$. Our calculations show that Co prefers to replace Mn^{3+} ion, rather than Mn^{4+} ion presented in the materials. This substitution improves the stability of the materials owing to decreasing the number of Mn^{3+} ions and the electronic conductivity is also enhanced. Thus, Co substitution into LMO compound enhances structural stability and electronic properties.

Keywords: Lithium-ion battery, cathode material, LMCO, first principles calculations, band structure analysis.

PP-23

SYNTHESIS, CHARACTERIZATION AND ENZYME INHIBITION STUDIES ON VARIOUSETHYL (8-hydroxy quinoline-7-yl)(quinoline-2-yl) methyl carbamate

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Abstract

In the present study, a novel non-phosgene process for the synthesis of Ethyl carbamates (EC) by a reaction of urea with ethanol was studied. The reaction between urea and ethanol was found to be a spontaneous reaction that took place in the absence of catalyst and gave EC as the main product. Addition of a catalyst markedly influenced the reaction behavior particularly basic catalyst (SiO_2-$NaHSO_4$) greatly enhanced the yield of EC. The mechanism of reaction and catalyst functioning was discussed. A series of derivatives of ethyl(8-hydroxy quinoline-7-yl)(quinoline-2-yl) methylcarbamate have been synthesized from 8- hydroxyl quinoline and quinoline -2-al. This product obtained was treated with copper and zinc acetate to get complexes. All newly synthesized compounds were characterized by UV, IR, EI-MS and H-NMR and then screened against acetylcholinesterase and butyrylcholinesterase enzymes. The results revealed that ethyl(8-hydroxy quinoline-7-yl)(quinoline-2-yl) methylcarbamate and its derivatives exhibited good inhibitory potential against acetylcholinesterase and butyrylcholinesterase and are possible target molecule for the treatment of Alzheimer's disease.

PP-24

ISOLATION, PHYSICO-CHEMICAL CHARACTERIZATION AND ANTI-MICROBIAL ACTIVITY OF 7-dimethylaminocinnamyl-8-hydroxyquinoline AND ITS TRANSLATION METAL COMPLEXES

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Abstract

A novel Mannich base of 8-hydroxyquinoline namely 7-dimethylaminocinnamyl-8-hydroxyquinoline(L) (DMACHQ) was synthesized by interacting dimethylamine, cinnamaldehyde and 8-hydroxyquinoline in 1:1:1 mole ratio at room temperature in chloroform medium. The brown coloured product was recrystallized using ethanol as solvent. The Manganese(II), Cobalt(II), Copper(II), Nickel(II), Zinc(II), Cadmium(II) and Mercury(II) complexes of DMACHQ were prepared by interacting the metal salts (Chloride) with the ligand (DMACHQ) in hot ethanol medium. They were isolated and structurally characterised by elemental analysis, conductance, magnetic susceptibility measurement, IR, Uv-Vis, NMR and Mass spectral data. The Mannich base ligand is found to chelate through the phenolic oxygen and the aliphatic tertiary amino nitrogen atoms. *Invitro* antimicrobial screening of the new Mannich base ligand and its metal complexes were carried out by employing Agar well diffusion technique. *E.Coli* and *S.aureus* were bacterial strains used wand *A.niger* and *P.chrysogenum* were fungi used. Streptomycin and Amphotericin-B were the standard antibiotic used to study the efficiency of the ligand and the complexes. The activities of the test compounds were compared with those of the standard drugs. It is found that they are effective against the microorganisms chosen for the study. The free ligand and metal complexes are having higher degree of activity than the standard drugs.

PP-25

PHYTOCHEMICAL ANALYSIS AND ANTIBACTERIAL STUDIES OF ETHANOLIC LEAF EXTRACT OF *ACALYPHA INDICA* HERBAL PLANT

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Abstract

Acalypha indica L. is one of herbal plants found in wet, moderate, tropical areas which grows as a weed. This herb has been used traditionally to treat dysentery, diarrhea, malnutrition, and malaria. But chemical compounds present in ethanolic extract of leaves of *Acalypha indica* L. hasn't been completely reported yet. The present study was extraction of pure compounds from leaf of Acalypha indica using ethanol and investigate the phytochemicals presence and antibacterial activity against the Gram negative bacterial strains of Salmonella typhi, Escherichia coli and Gram-positive bacterial strains of *Enterococcus faecalis* Bacillus cereus.

Key words: Acalypha indica L, Ehanol, Phytochemicals, Antibactrial activity

PP-26

SYNTHESIS OF THIOPHENE BASED CONJUGATED POLYMER AND ITS APPLICATION TO SUPERCAPACITORS

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Abstract

The storage of the energy resources in this technological world we live in, is at high stake. In order to store energy efficiently, researchers have been exploring new materials and

methods recently. The conversion and storage of energy for a constant supplication with special attention for storing electrochemical energy is highly in demand. Where Supercapacitors with high power density, quick charge–discharge time, low input resistance, extended cyclic stability are promising candidates to store electrical energy as solid-state device which may overcome many of the drawbacks in batteries. Thus, synthesis of new electrode materials with efficiency is considered to be paramount significance and order of the research retrospective literature survey reveals that in supercapacitors, organic conjugated polymers had displayed remarkable multifunctional characteristics. This research offers insight into the synthesis of Polythiophene-co-hexyloxybenzene (PTHOB). The as synthesised polymer was characterised using FT-IR and NMR spectroscopic techniques. Studies using cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectra (EIS) were conducted to investigate the electrochemical characteristics and capacitance of the same. Thus, the results of this material (PTHOB) shows specific capacitance of 443Fg^{-1} at current density 1Ag^{-1}, energy density 55.375 WhKg^{-1} and power density 450 WKg^{-1}. Since, this material (PTHOB) shows high perfomance this could be used as energy storage device.

PP-27

NOVEL OXALAMIDE-BASED FLUORESCENT SENSORS FOR Sn^{2+}/Fe^{3+} ions, GELATION PROPERTIES, AND THEIR UTILITY IN CELL IMAGING

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Abstract:

The development of colorimetric and fluorescence receptors *N¹*, *N²*-bis(2-piperazine-1-yl) ethyl)oxalamide [$OX(PIP)_2$] and Di-(benzoyloxalohydrazide) [$OX(BH)_2$] for the accurate and easy identification of Sn^{2+} & Fe^{3+} ions respectively in DMSO/HEPES buffer (1:9, v/v, 20 µM, pH 7.3) in the presence of other metal ions. The process of sensing entails the complexation of $OX(PIP)_2$ receptors with Sn^{2+} addition, which sets off the fluorescence 'Turn-On' mode and $OX(BH)_2$ displays 'Turn-Off' mode after the inclusion of Fe^{3+} ions. An improved linear correlation between fluorescence intensity and Sn^{2+}/Fe^{3+} concentration was attained in the range of 0−20 µM, with a detection limit (LOD) of 0.6 µM & 0.013 µM respectively. The average fluorescence lifespan measurements of $OX(PIP)_2$ and $OX(BH)_2$ were determined to be 2.77 and 2.22 ns and the average lifetime of 4.49 ns for $OX(PIP)_2 + Sn^{2+}$ and 2.18 ns for $OX(BH)_2 + Fe^{3+}$ were observed. The binding mechanisms of $OX(PIP)_2 + Sn^{2+}$ and $OX(BH)_2 + Fe^{3+}$ were confirmed by Fourier transform infrared analysis, NMR spectral titrations, and mass (ESI) spectral analysis. The chemosensing of $OX(PIP)_2$ and $OX(BH)_2$ has also been examined in bioimaging experiments as useful fluorescent markers for finding the source of Sn^{2+}/Fe^{3+} in living cells. Significantly, receptors $OX(PIP)_2$ and $OX(BH)_2$ could distinguish

Sn^{2+}/Fe^{3+} ions in live cells and Sn^{2+}/Fe^{3+} in human cancer cells.

Keywords: N^1,N^2-bis(2-piperazine-1-yl)ethyl)oxalamide, Di-(benzoyloxalohydrazide), Tin(II) ion, Iron(III) ion, TCSPC, Gelation, and MDA-MB-231 cell line.

PP-28

GREEN SYNTHESIS OF ZnO NANOPARTICLES FOR EFFICIENT BIODIESEL PRODUCTION

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Abstract

Biodiesel is suitable alternative candidate for conventional fossil fuels owing to biodegradable, non-toxic and renewable nature. Biodiesel harnessed from triglyceride rich sources such as vegetable oil (edible and non-edible), animal fat, and grease. Generally, biodiesel produced by catalytic transesterification or alcoholysis of triglyceride sources. In this study, ZnO nanoparticles was synthesized by co-precipitation method by using *Aloe barbadensis miller* (Aloe vera) leaf extract. The catalytic performance of the biosynthesized ZnO nanoparticles were demonstrated by transesterification of waste cooking oil as a low-cost feedstock. The influence of *Aloe barbadensis miller* extract also studied. The biosynthesized ZnO catalyst was characterized by XRD, FTIR, and SEM. The fatty acid ethyl ester (FAEE) phase in biodiesel sample studied by FTIR and it confirm the characteristic FAEE phase in prepared biodiesel sample. XRD revealed the phase composition and crystalline nature of the ZnO. SEM morphology revealed spherical like morphology with nanosized pores on surface and functional group were studied by FTIR.

Keywords: Zinc Oxide, Leaf extract, Transesterification, Biosynthesis

PP-29

BIOCOMPATIBLE BOROPHENE NANOSHEETS DECORATED WITH *NYCTANTHES ARBOR-TRISTIS* EXTRACT REDUCED SILVER NANOPARTICLES: BOOSTING ANTIBACTERIAL ACTIVITY

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Abstract

Borophene is a unique two-dimensional (2D) material with a single layer of boron atoms arranged in various structural phases depending on the growth conditions and substrate used during synthesis. Its unique properties, including high surface area, tunable electronic behaviour, and chemical reactivity, make it an intriguing candidate for biomedical and biotechnological applications. In the present work, silver nitrate ($AgNO_3$) was reduced with *Nyctanthes Arbor-Tristis* (*NAT*) extract to obtain silver nanoparticles (Ag NPs) and decorated on the surface of borophene sheets. Fabrication of Ag NPs (particle size = 7nm), involved the contribution of the Phyto-compounds in the *NAT*-extract which also functioned as reducing and stabilizing agents. Subsequently, *NAT*-Ag@borophene nanocomposites (NCs) structural, functional, and morphological behaviours was thoroughly investigated using FT-IR, XRD, Raman, FE-SEM and HR-TEM-SAED. The chemical composition and spin state were confirmed from EDX and XPS analysis. Interestingly, the synthesized *NAT*-Ag@borophene NCs exhibited high zone of inhibition for *S. aureus* (13 nm dia.) and *E. coli* (12 nm dia.) bacterial strains. Overall, the results were fruitful and provided insightful speculation that the *NAT*-Ag@borophene NCs material has the potential to be a wise substitute in the pharmaceutical and medical fields.

Keywords: Silver Nanoparticles; *Nyctanthes Arbor-Tristis*; Borophene Nanosheets; Antibacterial activity.

PP-30

SYNTHESIS OF SPINEL ZINC COBALT OXIDE NANOPARTICLES FOR PEROVSKITE SOLAR CELLS AND PHOTOCATALYTIC APPLICATIONS

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Abstract

Perovskite solar cells (PSCs) have emerged as a promising energy conversion device for efficient energy production. Currently, extensive research works have been directed towards enhancing the stability and performance of perovskite solar cells, with a focus on novel materials and device architectures. Additionally, photocatalytic degradation of organic dyes has significant attention in recent years due to its potential for wastewater treatment and environmental remediation. In both Perovskite Solar Cells and Photocatalytic applications, we have used spinel oxides due to its good thermal and chemical stability, which reduces the instability of the perovskite and also excellent catalytic behavior. In this study, the spinel zinc cobalt oxide ($ZnCo_2O_4$) nanoparticles were synthesized by hydrothermal method. The synthesized nanoparticles were characterized by X-ray Diffraction (XRD), Raman Spectroscopy, Field Emission Scanning Electron Microscopy (FE-SEM), High Resolution Transmission Electron Microscopy (HR-TEM) and X-Ray Photoelectron Spectroscopy (XPS) techniques. The PSCs was fabricated using the $ZnCo_2O_4$ as a composite with Perovskite ($CH_3NH_3PbI_3$) material. Photovoltaic performance of the fabricated device was investigated under one sun illumination. The photocatalytic behavior of $ZnCo_2O_4$ was studied by using the degradation of Congo red dye under Visible light irradiation. The results show that spinel $ZnCo_2O_4$ have excellent photovoltaic and photocatalytic performance.

Keywords: Spinel oxides, Zinc cobalt oxide, Photovoltaic performance, Photocatalytic degradation.

PP-31

SYNTHESIS AND CHARACTERIZATION OF CaO CATALYST FOR VEGETABLE OIL TRANSESTERIFICATION

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Abstract

Biodiesel is a renewable and environmentally friendly substitute to conventional diesel fuel. Biodiesel has gained significant interest owing to its potential to mitigate greenhouse gas emissions and reduce dependence on fossil fuels. Biodiesel, a fuel that burns cleanly, is derived from grease, vegetable oils, or animal fats. It is obtained through the process of transesterification, where oils are reacted with short-chain alcohols, or by esterification of fatty acids. The transesterification process involves the conversion of triglycerides to fatty acid alkyl esters. This reaction takes place in the presence of an alcohol, such as methanol or ethanol, and a catalyst, which can be either an alkali or acid. In this study, biosynthesis of CaO nanoparticles was carried out through co-precipitation method by using *Carica papaya* leaf extract as capping agent. The CaO synthesized through biological processes was successfully employed in the transesterification of *Sesamum indicum* (sesame) seed oil, resulting in the production of biodiesel. The physicochemical characteristics of the synthesized CaO nanoparticles was performed using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). Analysis of the biodiesel sample by FTIR revealed the presence of the Fatty Acid Ethyl Ester (FAEE) phase which confirms the successful biodiesel production. This study identified calcium oxide (CaO) as a promising catalyst for converting *Sesamum indicum* oil into biodiesel through transesterification.

Keyword: Biodiesel, Transesterification, Calcium oxide, Biosynthesis

PP-32

Synthesis of Nanostructured Oxide Materials for Highly Efficient Pseudocapacitor

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Abstract

Supercapacitors also known as electrochemical capacitors have emerged as promising energy storage devices due to their high-power density, fast charging-discharging rates, and long cycle life. Various electrode materials have been explored for supercapacitors like transition metal oxides, metal sulfides, metal selenides and carbon materials. Among them, transition metal oxides have emerged as promising candidates due to their favourable electrochemical properties and abundance. Transition metal oxides such as Manganese Oxide (MnO_x), Nickel Oxide (NiO_x), Cobalt Oxide (CoO_x), Vanadium pentoxide (V_2O_5) and Tungsten trioxide (WO_3) have attracted considerable attention due to their excellent electrochemical properties. In recent years, nanocomposite materials combined with V_2O_5 and WO_3 have shown greater potential for enhancing the performance of supercapacitors. Metal oxide nanocomposites have good pseudocapacitive behaviour. In this work, we have prepared V_2O_5/WO_3 nanocomposites that were synthesized by hydrothermal method. The synthesized material was characterized by using X-ray diffraction (XRD), Raman Spectroscopy, UV-VIS spectroscopy and Scanning Electron Microscopy (SEM). Cyclic Voltammetry, Galvanostatic Charge-Discharge tests and Electrochemical Impedance Spectroscopy were used to evaluate the electrochemical performance of synthesized nanocomposites. The nanocomposite of V_2O_5/WO_3 material shows the better specific capacitance and superior stability. These obtained results highlight the possibility of the hydrothermally produced V_2O_5/WO_3 nanocomposite as an electrode material for supercapacitor applications, opening the door for the construction of high-performing energy storage devices.

Keywords: Supercapacitor, Hydrothermal method, Nanocomposite, Cyclic voltammetry.

PP-33

FABRICATION OF HIGHLY STABLE AND EFFICIENT PEROVSKITE SOLAR CELLS USING NiO/MWCNT INCORPORATED $CH_3NH_3PbI_3$

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Abstract

In recent years, perovskite solar cells (PSCs) have attracted great attention among the photovoltaic researchers owing to its facile fabrication and higher power conversion efficiency of up to 25.7%. The inorganic hole transport material offers a greater advantage to PSCs. But the inorganic hole transport materials have challenges to deposit uniformly on the perovskite layer because of their poor dispersibility in non-polar solvents, which restricts the ability to obtain the efficient and stable PSCs. In this work, Nickel Oxide/Multi-wall Carbon Nanotube (NiO/MWCNT) composites have been synthesized by hydrothermal method and are directly incorporated with $CH_3NH_3PbI_3$ to increase the performance of PSCs with stability. The incorporation of NiO/MWCNT improves the properties of $CH_3NH_3PbI_3$ such as formation of large grain size/grain boundaries, minimal defects, enhanced charge generation/collection and reduced recombination. The NiO/MWCNT- $CH_3NH_3PbI_3$ based PSCs exhibited the higher power conversion efficiency (PCE) of 14.91% with a J_{sc} of 24.77 mA/cm^2, V_{oc} of 0.97 V and FF of 0.62, which is significantly higher PCE than that of bare device. The higher charge carrier recombination resistance was observed from the electrochemical impedance spectroscopy, which evinces the low recombination in the NiO/MWCNT- $CH_3NH_3PbI_3$ based PSC. The low recombination and large grain in the $CH_3NH_3PbI_3$-NiO/MWCNT film were confirmed by the strong photoluminescence (PL) quenching effect and red shift of the PL spectrum. The NiO/MWCNT incorporated PSC reduced only 6% of its initial PCE after 600 hours of aging under room atmosphere whereas the PCE of bare device reduced 13% of its initial PCE value. Moreover, the carbon was used as a back electrode to increase the stability and reduce the fabrication cost of PSC.

Key words: Perovskite Solar Cell, NiO/MWCNT-$CH_3NH_3PbI_3$, Hydrothermal method.

PP-34

GREEN ROUTE SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF CHITOSAN/MgO COMPOSITE AND ITS APPLICATION AS ANTIBACTERIAL AGENT

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Abstract

Currently, green synthesis approaches are gaining much attention among researchers for the synthesis of nanoparticles. Furthermore, the rise of prevalent bacterial diseases has generated a growing concern for biopolymer coated composite materials. In this report, chitosan-based magnesium oxide (CS-MgO) composite has been effectively formulated via green synthesis using the *Eucalyptus globulus* extract (EGE), by treating the chitosan as biosurfactant. The *EG* leaf extract can serve as a perfect reducing agent comprising lot of bioactive components. Then, the functional groups of the synthesized composite was characterized the by FTIR analysis. UV-Vis spectroscopy was used to confirm the formation of the nanoparticles. Thermal stability was studied by TGA analysis and SEM analysis was done to inspect the morphology of the composite. The X-ray diffraction (XRD) technique was utilized to demonstrate the crystalline nature and size of the nanoparticles. The antibacterial activity was tested against gram positive (*S.aureus*) and gram negative (*E.coli*).

Keywords: Chitosan, MgO, *Eucalyptus globulus* extract, Antibacterial activity.

PP-35

$AgMoO_4$/CARBON COMPOSITES: NOVEL BIFUNCTIONAL MATERIALS FOR SUPERCAPACITOR APPLICATION

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Abstract

$AgMoO_4$/Carbon composites represent a promising class of materials for supercapacitor applications, offering a unique combination of properties conducive to efficient energy storage. $AgMoO_4$ was synthesized hydrothermal route and it composites exhibited enhanced specific capacitance and excellent cycling stability, and improved conductivity. The influence of carbon morphology, synthesis parameters, and composite structure on the electrochemical performance of $AgMoO_4$/Carbon composites is addressed in this work. Furthermore, the underlying mechanisms governing charge storage in these composites are explored, shedding light on their potential as bifunctional materials for supercapacitor devices.

Keywords: AgMoO4, Carbon composites, Supercapacitors, Bifunctional materials, Hydrothermal synthesis, Charge storage

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PP-36

FABRICATION OF BINARY COMPOSITE NiO/CuO AS AN ELECTRODE MATERIAL FOR HIGH-PERFORMANCE SUPERCAPACITORS

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Abstract:

The supercapacitor, which has been attracting growing interest in energy-storage applications since the past decade, is an alternative that evinces the potential to emulate future battery technology. Numerous studies have been conducted on metal-based compounds and their composites. However, the real specific capacitance value of NiO electrodes greatly depends on their morphology, surface area and pore properties, which influence its practical use in supercapacitors. In order to improve the electrochemical properties of NiO, many NiO-based nanocomposites have been designed and fabricated for high-performance supercapacitors. In this work NiO-CuO nanocomposite was synthesized using simple co-precipitation method and used as a high-performance supercapacitor electrode by using surfactant. Electrochemical tests showed that NiO-CuO displayed good capacitance behaviour. Furthermore, increasing the surfactant ratio helps to enhance the capacitance property. The precise characterization of composite was analyzed by XRD, TEM and electrochemical studies. This work proposes that the improved electrochemical properties can be obtained using surfactant consists of transition metal oxides.

Keywords: Co-precipitation; NiO; CuO; Supercapacitor.

PP-37

SYNTHESIS AND CHARACTERIZATION OF YTTRIUM DOPED TiO_2 NANOPARTICLES FOR PHOTOCATALYTIC APPLICATIONS

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Abstract:

Water pollution is a major issue that has garnered the attention of researchers. The contamination of water occurs due to various factors such as domestic, industrial, agricultural, scientific, and technological activities. The textile industry is the primary contributor to the release of wastewater with dye into the environment. Photocatalysis is a promising technique to mitigate the water pollution. Titanium dioxide nanoparticles (TiO_2 NPs) are promising photocatalytic materials for the photodegradation of organic dyes in wastewater. In this work, bare TiO_2 and Yttrium doped TiO_2 nanoparticles were synthesized by sol-gel technique. For analysing the catalyst, X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM), and UV visible spectroscopy techniques were used. The photocatalytic activity of the bare TiO_2 and Yttrium doped TiO_2 was studied by the degradation of rhodamine B dye under Visible, UV light, and direct solar light. Yttrium doping improve the photocatalytic activity and demonstrated the higher photodegradation efficiency compared to that of bare TiO_2. The obtained result shows that the yttrium doping has a crucial impact on the photocatalytic behavior.

Keywords: Photocatalytic degradation, Sol-Gel Method, Yttrium doped TiO_2, Rhodamine B

PP-38

SYNTHESIS AND CHARACTERIZATION OF ALUMINIUM VANADATE/POLYPYRROLE COMPOSITE FOR SUPERCAPACITOR APPLICATION

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Abstract

Aluminium vanadate, a transition metal oxide, exhibits high specific capacitance and stability, rendering it promising for supercapacitor electrodes. When integrated with polypyrrole, a conducting polymer, the resulting composite materials display improved electrical conductivity, enhanced surface area, and superior electrochemical performance. $AlVO_4$/PPy composites were synthesized by hydrothermal method. The morphology, and structure of $AlVO_4$/PPy composites were examined by scanning electron microscopy. The resistance of this composite was evaluated by impedance studies. The extensive work on charge-discharge studies helps to tailor the capacitance behaviour of proposed composites. This work provides the optimization of these composite materials $AlVO_4$/PPy for practical energy storage applications.

Keywords: Aluminium vanadate, Polypyrrole, Hydrothermal method, Electrochemical Studies

PP-39

SYNTHESIS OF SILVER DOPED TiO_2 NANOPARTICLES FOR PHOTOCATALYTIC APPLICATIONS

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Abstract

Photocatalysis is the best potential technology to replace conventional wastewater treatment methods due to its utilization of visible light to degrade organic and inorganic pollutants. Nobel metal doping has emerged as an effective method for improving the activity of TiO_2. The localized surface plasmon resonance (LSPR) effect of noble metals facilitates TiO_2 photocatalysts to enhance the excitation of electrons at the catalyst surface. It also increases the lifetime of electron and hole pairs, which increases the photocatalytic efficiency of TiO_2. In this study, Silver (Ag) doped- TiO_2 NPs was used for photocatalytic application. Ag doped- TiO_2 has high stability and maintains its high degradation efficiency to apply them for several applications such as the removal of dyes, other water pollutants, microbes, and metals. Different concentrations of Ag doped- TiO_2 have been synthesized by the sol-gel route. The characterization was done by X-ray diffraction (XRD), Scanning electron microscopy (SEM), and Ultraviolet-Visible Diffuse Reflectance Spectroscopy (UV-Vis DRS). The photocatalytic activity of bare TiO_2 and Ag- TiO_2 was evaluated by measuring the degradation of Rhodamine B (RhB) dye under visible, direct solar light, and UV light irradiation. The experimental result for Ag doped- TiO_2 indicates the very high degradation up to 96.5%, 10%, and 98.7%, under visible, dark, and UV light radiation, respectively. The photocatalytic efficiency of Ag-TiO_2 was better than the bare TiO_2 for the photodegradation of Rhodamine B.

Keywords: Photocatalysis, Ag-doped TiO_2 Nanoparticles, Sol-gel method, Degradation of Rhodamine B

PP-40

SYNTHESIS OF Mn_3O_4-ZNO NANOCOMPOSITE FOR PHOTOCATALYTIC DEGRADATION OF DYES

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Abstract

The Photocatalysis is a low-cost, sustainable, and environmentally acceptable method for treating wastewater. In recent years, dyes have been used extensively in the textile sectors, paper and leather industries. The dyes are hazardous and affects all the living things. In this work, Mn_3O_4-ZnO nanocomposite was prepared and used for degradation of organic pollutants. Mn_3O_4-ZnO nanocomposite (80-20%, 60-40%, 50-50%, 40-60%, and 20-80%) was synthesized via a facile microwave method. Mn_3O_4-ZnO nanocomposite is low cost, naturally abundance, environmentally friendly and has interesting photocatalytic performance. Then, the prepared catalyst was analyzed by advanced instrumentation techniques such as XRD, SEM, EDAX, UV-DRS. The catalyst activity of the catalyst was studied by the degradation of rhodamine B, and Congo red under visible light. The degradation rate of the dye was studied, and results will be discussed.

Keyword: Mn_3O_4- Zno Nanocomposite, Microwave method, Rhodamine B and Congo r

PP-41

POLYSILOXANE-BASED CHOLESTERIC SIDE-CHAIN LIQUID CRYSTAL ELASTOMERS CONTAINING DIFFERENT CROSS-LINKERS

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Abstract

Side-chain liquid crystal elastomers (LCEs) containing a common cholesteric monomer but different cross-linkers (CLs) are described. These polysiloxane-based elastomers were synthesized following a hydrosilylation reaction in which a vinyl-terminated monomer and divinyl-terminated CL were appended to polymethylhydrosiloxane backbone in presence of a platinum catalyst [1]. Four such elastomers were synthesized by varying the CLs-an alkyl CL, a phenyl-containing CL, a biphenyl-based CL and an azobenzene containing CL. Thermal, mesomorphic properties, swelling behavior, mechanical and actuation properties of the elastomers are discussed. The LCE containing azo-CL displayed wider phase range, low cross-link density and noticeable actuation compared to other elastomers [2].

Keywords: Liquid crystal elastomer,cross linker, actuation.

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PP-42

ULTRASONIC ASSISTED SYNTHESIS OF IRON OXIDE AND CALCIUM CARBONATE DECORATED POLYPYRROLE FUNCTIONALIZED REDUCED GRAPHENE OXIDE FOR SUPERCAPACITOR APPLICATION

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Abstract

Green energy sources such as Solar energy are often constrained by lack of sufficient energy storage. Electricity produced from renewable energy sources have to be efficiently stored to meet the demands of the society. One of the leading energy storage techniques to meet the current energy demands is Supercapacitor. The aim of our study is to achieve a material of high electrical conductivity, large storage capacity, high cyclic stability using reduced graphene oxide (rGO) which has good porosity and large surface area. To enhance the electron transfer process the conducting polymer polypyrrole (Ppy) is functionalized on rGO. Further, to increase the storage capacity of the composite, transition metal oxides could be efficient due to their variable valence states and high electrical conductivity. Fe_2O_3 and $CaCO_3$ are decorated on Ppy-rGO by simple ultrasonication method in which Fe_2O_3 possess the ability to store the synthesized ternary nanocomposite $Fe_2O_3/CaCO_3$@Ppy-rGO stores charge through faradaic process and behaves as a pseudo capacitor to address the low energy density and achieve high power density. The electrochemical characteristics of the ternary nanocomposite were examined using Cyclic Voltammetry, Galvanostatic Charge Discharge, Electrochemical

Impedance spectroscopy and Tafel plot. The ternary nanocomposite has shown fast charging and slow discharging behavior and exhibited a high specific capacitance in a current density of 1A/g.

PP-43

INFLUENCE OF CELLULOSE NANOCRYSTALS ON STRENGTH OF MAIN-CHAIN LIQUID CRYSTAL ELASTOMERS

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Abstract

Liquid crystal elastomers (LCEs) are one such soft actuator which exhibit a spontaneous reversible deformation (large actuation stroke) in response to external stimuli and have shown great potential for applications in many fields namely mechanical actuators, artificial organs, smart surfaces.[1] Multi-stimuli responsive LCEs (for example sensitive to light, electric and magnetic field) having better performances can be obtained through incorporation of other materials such as nanoparticles, inorganic conductive thermal fillers etc.[2] In this regard we propose cellulose nanocrystals (CNCs) as ideal nanofillers in LCEs to enhance the properties of main-chain LCEs. CNCs were prepared through the standard acid hydrolysis method. The main-chain LCE was prepared using a two-stage thiol-acrylate Michael addition followed by a photo-polymerization reaction using an acrylate monomer, a dithiol, a tetra thiol, a base catalyst, and a photo initiator. Different wt% of CNCs were incorporated during the preparation of the elastomer to obtain the composites and the influence of the CNCs on the mechanical, elastic, and actuation properties of the composites was studied. As expected, the inclusion of CNCs indeed improved the mechanical properties, however, until a threshold value. On further increasing the amount of CNCs was found have a negative impact. More interestingly, the elastic properties of the composite materials were found to be intact and the elastomeric films displayed remarkable thermal actuation.

Key Words: Cellulose nanocrystals, liquid crystal elastomer, filler, elastic, thermal actuation.

PP-44

ANALYSIS OF SILVER NANOPARTICLES PREPARED FROM HIBISCUS ROSA-SINENSIS LEAF EXTRACT THROUGH GREEN SYNTHESIS METHOD

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Abstract

The development of simple, nontoxic and eco-friendly method for the preparation of nanoparticles is an important step in the field of nanotechnology. Among the metallic nanoparticles, silver nanoparticles (AgNPs) gain much attention due to its chemical, physical and biological properties and applications. This study was carried out by synthesis and characterisation of silver nanoparticle using a composite leaf extract of Hibiscus Rosa-Sinensis. Various molecules (alkaloids, polysaccharides, alcoholic compounds, vitamins and amino acids) present in plant have ability to bio-reduction, formation and stabilization of silver nanopoarticles. The synthesis and characterization of silver nanoparticles was confirmed by UV-Visible spectrophotometer, Fourier Transform Infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM). UV-Visible absorption spectra of the reaction medium containing silver nanoparticles showed maximum absorbance at 401 nm. FTIR analysis confirmed reduction of Ag^+ ions to Ag^0 ions in synthesized silver nanoparticles. The SEM analysis showed the particle size between 1-50 nm and polydispersed spherical in structure. This study revealed that the compounds from the extracts of *Hibiscus rosa-sinensis* L. are good reducing and stabilizing agents for the synthesis of silver nanoparticles.

KEYWORDS: Hibiscus rosa-sinensis, Silver nanoparticles, UV, FTIR, SEM, EDS.

PP-45

BIOACTIVE IMINE DERIVATIVE OF LAWSONE AND ITS METAL COMPLEXES: PREPARATION, CHARACTERIZATION, *in vitro* AND *in silico* BIOLOGICAL EVALUATION

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Abstract

This article is concentrated on the imine derivative of lawsone which is prepared using 3-amino 1,2,4 triazole. Four metal complexes [Co(II), Ni(II), Cu(II) and Zn(II)] have been synthesized using this imine derivative as the primary ligand. A few articles have been focused on the imine derivatives of lawsone which are formed in specific conditions unlike other Schiff bases. The prepared compounds are characterized by techniques such as UV-Vis, IR, NMR, Mass and EPR. All these methods confirm the presence of imine group and the octahedral geometry of the complexes. The prepared complexes are assessed for their DNA binding properties which confirm that the binding mode is intercalative. The biologically potential ligand and its complexes also exhibit distinct pharmacological activities such as antioxidant and antimicrobial activities against bacteria such as *B.subtilis, S.aureus, E.coli* and *S.typhi,* and

fungi such as *A.niger, A.flavus, C.albicans and R.bataticola*. The antioxidant assay was examined through DPPH assay. Besides, the compounds are scrutinized for their DFT studies using Gaussian 09 programme. Various reactivity descriptors are calculated based on the HOMO-LUMO energies. Molecular docking is conducted with two different receptors 1BNA and 1HD2 proteins to obtain a deeper understanding on the *in vitro* DNA-binding, anti-oxidant assay results and also the interaction of the compounds with different proteins.

PP-46

LIQUID CRYSTAL ELASTOMER-POLYANILINE COMPOSITE FILMS FOR IR ACTUATION

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Abstract

Artificial muscles are becoming increasingly popular due to the rapid advancements in machine intelligence and human-machine interactions, as well as their vast potential for use in biomedical and soft robotics applications. This study detailed and proved the muscle-like actuation and weight-lifting capabilities of composite materials made of liquid crystal elastomer (LCE) and polyaniline (PANI)-doped LCE. The PANI is prepared using the chemical reduction method [1]. The LCE and LCEs doped with different concentrations of PANI were prepared using the thiol-Michael addition click chemistry approach [2]. All the films exhibited reversible thermal and photoactuation with excellent weight-lifting capabilities. Interestingly, the doped films exhibited intriguing self-healing characteristics in addition to exceptional contraction, expansion, and rotation in response to photostimuli. All these characteristics strongly highlight the suitability and potential of the prepared films for application as artificial muscles.

Keywords: Liquid crystal elastomer, Polyaniline, Photothermal Actuation, Mechanical property.

PP-47

ISOLATION, PHYSICO-CHEMICAL CHARACTERIZATION AND ANTI-MICROBIAL ACTIVITY OF 7- DIMETHYLAMINOCINNAMYL-8-HYDROXYQUINOLINE AND ITS TRANSLATION METAL COMPLEXES

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Abstract

A novel Mannich base of 8-hydroxyquinoline namely 7-dimethylaminocinnamyl-8-hydroxyquinoline(L) (DMACHQ) was synthesized by interacting dimethylamine, cinnamaldehyde and 8-hydroxyquinoline in 1:1:1 mole ratio at room temperature in chloroform medium. The brown coloured product was recrystallized using ethanol as solvent. The Manganese(II), Cobalt(II), Copper(II), Nickel(II), Zinc(II), Cadmium(II) and Mercury(II) complexes of DMACHQ were prepared by interacting the metal salts (Chloride) with the ligand (DMACHQ) in hot ethanol medium. They were isolated and structurally characterised by elemental analysis, conductance, magnetic susceptibility measurement, IR, Uv-Vis, NMR and Mass spectral data. The Mannich base ligand is found to chelate through

the phenolic oxygen and the aliphatic tertiary amino nitrogen atoms. Invitro antimicrobial screening of the new Mannich base ligand and its metal complexes were carried out by employing Agar well diffusion technique. E.Coli and S.aureus were bacterial strains used wand A.niger and P.chrysogenum were fungi used. Streptomycin and Amphotericin-B were the standard antibiotic used to study the efficiency of the ligand and the complexes. The activities of the test compounds were compared with those of the standard drugs. It is found that they are effective against the microorganisms chosen for the study. The free ligand and metal complexes are having higher degree of activity than the standard drugs.

PP-48

Co-GRAFTED IMINE FUNCTIONALIZED MCM-41 AS EFFICIENT AND REUSABLE CATALYST FOR THE SYNTHESIS OF TETRAKETONES VIA KNOEVENAGEL CONDENSATION

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Abstract

A new type of Co-Complex exogeneous Schiff base ligand immobilized on MCM-41 has been synthesized. In order to elucidate the morphology, pore structure, and surface properties of the newly prepared catalyst was characterized by FT-IR, SEM-EDX, TGA, ICP-OES, PXRD and ^{13}C-CP-MAS-NMR. Our synthesized catalyst has been found more active, efficient and promising one for Knoevenagel Condensation in EtOH/H_2O medium under ultrasonication. Furthermore, the performance of the catalyst was enhanced by the synergistic effect due to the presence of both imine and exogeneous ligand together. Thus, the MCM-41 binded heterogeneous catalyst have remarkably active, stable, recoverable and reusable.

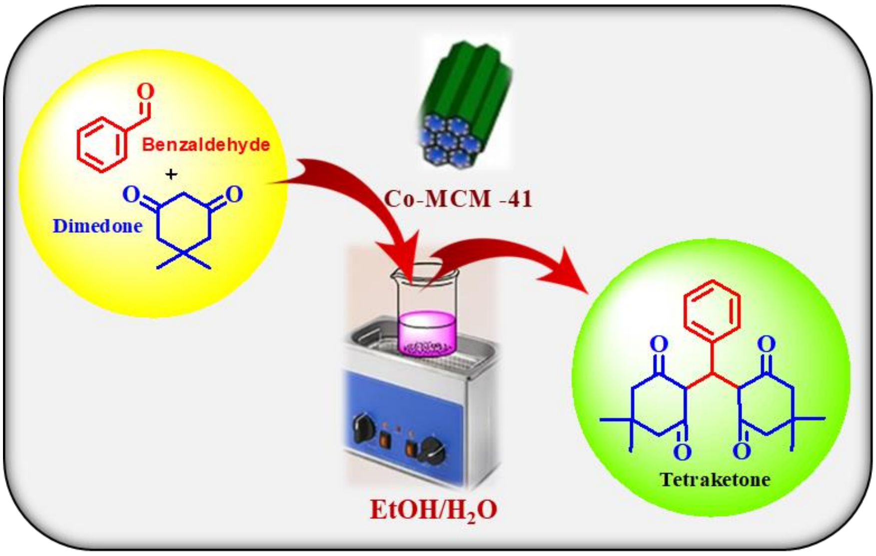

Fig 1: Synthesis of Tetroketones via Knoevenagel Condensation

Keywords: Heterogenous catalyst, MCM-41, Knoevenagel Condensation.

PP-49

ANALYSIS OF BIOGAS PRODUCTION FROM DAIRY MANURE USING AUTOMATIC METHANE POTENTIAL TEST SYSTEM

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Abstract

Biogas generation from organic residues is a well-established technology. Cow dung has a high methane content, typically around 55-70%, which makes it a suitable substrate for biogas production. Cow dung is rich in organic matter and nutrients, such as nitrogen and phosphorus, which can enhance the biogas production process and improve the quality of the digestate. The residue left after biogas production which can be used as a fertilizer. In this study, the production of methane of cow dung was found in the range of 2640.3Nml, 2416.4Nml, 6982.2Nml ,7377Nml which was determined using Automatic Methane Potential Test System II. Additionally, this research delves into the discussion of various type of waste and the necessary criteria for their inclusion in anaerobic digestion. The methane potential of various organic substrates was assessed using the test system under anaerobic conditions.

Keywords: Anaerobic digestion, biogas production, biodegradable waste, AMPTS II

PP-50

DECORATION OF DELAFOSSITE PHASE $CuCo_2O_4$ MATERIAL ON N-DOPED HOLLOW CARBON SPHERE AS AN ELECTROCATALYST FOR NEUROTRANSMITTER SENSING

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Abstract

This work describes the state of the art of electrochemical devices for the detection of an important class of neurotransmitters.There are many types of NTs in the brain, including epinephrine, norepinephrine (NE), dopamine, and glutamate. Researchers have focused on the role of serotonin molecules within the human body because they are involved in many important biological functions and are commonly associated with several diseases, such as Alzheimer's, Parkinson, depression, memory loss. Electrochemical sensors have attracted the attention of researchers as they possess high sensitivity, quick reaction rate, good controllability, and instantaneous detection. Efficient complex materials provide considerable benefits for biological detection as they have exclusive chemical and physical properties. Due to distinctive electrocatalytic characteristics, metallic nanoparticles add fascinating traits to materials that depend on the material's morphology and size. With respect to sensor application investigations, hollow mesoporous carbon sphere- based materials of the delafossite type of

copper and cobalt oxide ($CuCo_2O_4$), which is ABO_2 type material and heteroatom – doped materials are gaining popularity. Mesoporous hollow carbon material is highly crucial for high performance sensors. In this work, bimetal oxides decorating delafossite on N-doped hollow carbon sphere materials ($CuCo_2O_4$@NHCS) with high surface area and large volume achieved by a straightforward single step polymerization procedure followed by carbonization temperature is 900 °C .Where dopamine hydrochloride (DA) and Tetraethyl ortho silicate (TEOS) were used as C,N and silica precursor, while both are involved in silica–poly dopamine (PDA) sphere formation followed by cobalt acetate tetrahydrate and copper acetate monohydrate were added to PDA mixture. Then procedure followed by removing silica by the hard template method etching to $CuCo_2O_4$@NHCS. Among the $CuCo_2O_4$@NHCS material exhibit improved surface area, porosity and layer thickness. A sensitive electrochemical sensor for the determination of serotonine has been introduced.

PP-51

FABRICATION AND EVALUATION OF 2D MATERIALS-BASED SUPERCAPACITORS

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Abstract

Supercapacitor is a promising energy storage device with rapid charging and discharging cycles that contribute to the rapid growth of applications ranging from low power electronics like wearable, portable electronic devices to high power defence applications. This work delves into the comprehensive fabrication, characterization, and evaluation of supercapacitors by using hydrothermally synthesised Molybdenum Disulphide-reduced Graphene Oxide (MoS_2-rGO) nanocomposite as an active electrode material. The observed increase in specific capacitance with decreasing scan rate indicates the materials potential suitability for applications in supercapacitors. The morphological and structural aspects were investigated through atomic force microscopy (AFM), laser confocal microscope for GO, X-ray diffraction (XRD), Raman spectroscopy and Scanning Electron Microscopy (SEM). The surface topography and roughness were analysed using SEM and it confirms the well-dispersed and interconnected nature of MoS_2-rGO within the electrode material. The specific capacitance of 737.878 F/g was obtained for the MoS_2-rGO nanocomposite.

Keywords: Supercapacitor, MoS_2-rGO nanocomposite, Hydrothermal method.

PP-52

SYNTHESIS, CHARACTERIZATION AND ELECTROCHEMICAL PROPERTIES OF FLUORINATED CHITOSAN FOR BIOMOLECULAR SENSOR PLATFORM APPLICATION

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Abstract

Surface engineering of carbohydrate materials for biomedical application has huge market potential by product types such as biosensor platform, anti-microbial agents and thin film for water treatment. Chitosan (CS) a marine derived carbohydrate (biopolymer), is promising healthcare material owing to its biocompatibility, biodegradability, and ease surface functionality. Herein, CS is conjugated with pentafluoropropionic anhydride *via* Schiff base reaction to form fluorinated CS (CSF) and demonstrated for electrochemical biomolecular sensing of Hispidin, fungal metabolite / drug and luminescence active biomolecule. The structural integrity between CS and pentafluoropropionic anhydride has been comprehensively studied using FTIR, Raman and NMR spectroscopy. Cyclic voltammogram of CSF modified glassy carbon electrode (GCE) exhibits better electron transfer kinetics in potassium ferri/ferrocyanide electrolyte condition following a surface confined process. The electrochemical behaviour of hispidin depicts a reversible redox behaviour ($2e^{-}/2H^{+}$) at phosphate buffered saline (pH 7) electrolyte. Chronoamperogram based Hispidin detection exhibits a linear detection range of 10-250 µM using the CSF modified GCE. Sensing parameters such as selectivity, sensitivity, limit of detection and quantification of the prepared CSF electrode material against target, Hispidin is under progress, which will open new avenues in biomolecular sensor platform.

PP-53

FABRICATION OF DRUG LOADED CHITOSAN/SERICIN COMPOSITE FILM; INVITRO CYTOTOXICITY AND ANTIBACTERIAL ANALYSIS AND BIOCOMPATIBILITY EVALUATION

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Abstract

To overcome the drawback of the drawback of the biopolymer by integrated of polymer blending. The compatibility of biopolymer blends with incorporation of drugs within polymer matrices to enhance physicochemical properties and significant attention in biocompatibility, biodegradability. The composite of surface adhesive film prepared by solution casting method. An alkaline polysaccharide of chitosan (CS) blended with a resilient fibrous protein, silk fibroin (SF) composite film surface possesses the ability to attract and bind silver ions, thereby encouraging their transformation into silver nanoparticles (AgNPs) through reduction process. Antimicrobial resistant drug of ibuprofen integrated in the composite of CS/SF/Ag enhanced the ability towards the pathogenic microorganism. Swelling behavior of composite film improve the hydrophilicity with a contact angle of 98.1° to control the releasing of AgNPs /IBF sustained drug delivery by the polymer swelling kinetics mechanism followed fickian diffusion model. The film effectively combats bacteria *E. coli* and *S. aureus*, with zone of inhibition measurements of 11.5±0.14 mm and 10±0.12 mm, 80% inhibitory effect of antibiofilm activity against gram-positive bacteria by long lasting releasing of blended materials. The results indicated that AgNPs/IBF have strong anti-bacterial and anti-biofilm activity against the examined pathogens. Therefore, the composite of CS/SF/Ag/IBF film for target drug delivery system and potentially used in biomedical applications.

Keywords: Chitosan, Silk fibroin, Ibuprofen, pH response, Drug release kinetics.

PP-54

A GREENER APPROACH: *TRIGONELLA FOENUM-GRAECUM*-ASSISTED SILVER NANOPARTICLE DECORATED ON SILICENE NANOSHEETS FOR ENHANCED BIOLOGICAL ACTIVITY

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Abstract:

A distinctive, environmentally conscious, and sustainable pathway for biosynthesis of silver nanoparticles (AgNPs)-anchored silicene platform for biological application. However, the design of silicene-based composites for multifunctional medicinal applications remains a complex and challenging task. In this study, thin-layered silicene nanosheets (11 nm) composed of coordination-deficient metal atoms was synthesized via a liquid phase exfoliation technique. Subsequently, reduced Ag NPs (7-9 nm) with *Trigonella Foenum-Graecum* (*TFG*) seed extract were incorporated into silicene nanosheets and used for inhibiting the bacterial cell proliferation. The bio-fabricated Ag/silicene sheets were characterized using UV-visible, FT-IR, FE-SEM, HR-TEM and XRD analysis. Notably, the antibacterial assay (disc diffusion method) results suggest that the composite delivered a superior inhibited zone value of 21 nm and 22 nm against S. aureus and E. coli bacterial strains. Eventually, better antibacterial activity was due to the enhanced specific surface area (234 m^2/g) of silicene nanosheets, synergism between bioactive components in *TFG* seed extract and Ag NPs. This formulation offers numerous reaction sites for generation of ROS species that promotes bacterial cell lysis effectively. Henceforth, the *TFG* assisted Ag/silicene nanosheets could function as an effective coating for inhibiting antibacterial growth on bone implants via promoting osteogenesis.

Keywords: Antibacterial activity, *Trigonella Foenum-Graecum;* Silver Nanoparticles; Silicene Nanosheets;

PP-55

SYNTHESIS OF RARE EARTH MOLYBDATE@ACTIVATED CARBON NANOCOMPOSITE FOR THE ELECTROCHEMICAL DETERMINATION OF THEOPHYLLINE

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Abstract

We developed Dysprosium Molybdate@Activated Carbon (Dy_2MoO_6@AC) nanocomposite by a simple preparation method for the electrochemical determination of Theophylline (TP). The crystallographic phase, functional groups, surface analysis, and elemental distribution were examined using XRD, FT-IR, HR-TEM and EDS spectroscopic techniques respectively. The electrochemical characteristics were performed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) differential pulse voltammetry (DPV), and amperometric (i-t) techniques. Dy_2MoO_6@AC/GCE shows more enhanced electron transport property, higher surface area and more efficient electrocatalytic activity towards Theophylline (TP).

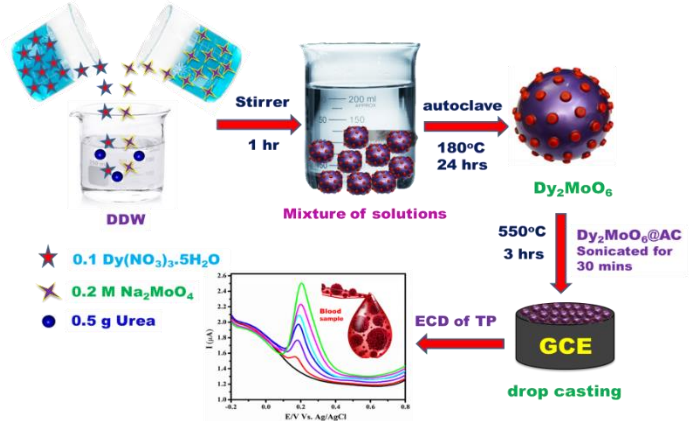

Figure : Schematic representation of the synthesis and fabrication of Dy_2MoO_6@AC nanocomposite.

Keywords: Dysprosium Molybdate, Activated Carbon, Electrochemical sensor and Theophylline.

PP-56

HYDROTHERMAL SYNTHESIS OF YTTERBIUM MOLYBDATE NANOPARTICLE FOR THE ELECTROCHEMICAL DETECTION OF L-DOPA

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Abstract

Being a critical neurotransmitter, L-dopa has been effectively used in the treatment of Parkinsons disease. In this study, we developed a simple bimetallic nanoparticles, Ytterbium Molybdate **(**$YbMoO_4$) using hydrothermal followed by calcination method. The formation of $YbMoO_4$ nanoparticle was confirmed using UV, FTIR and XRD analysis. The electrochemical behaviour of L-dopa was performed by using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV) techniques. This nanoparticle has been utilized as an electrochemical sensor for the electro oxidation of L-Dopa. Hence the developed sensor provides the enhancement in the peak current and shift in the oxidation potential towards negative direction. Due to $YbMoO_4$ nanoparticle's higher surface area and better catalytic activity, it show low detection limit of 0.7027 µM and higher sensitivity 158.32 $\mu A\ \mu M^{-1} cm^{-2}$ towards the detection of L-Dopa . It shows that the $YbMoO_4$/GCE is a good electrochemical sensor for the highly sensitive detection of L-Dopa.

Keywords: Ytterbium molybdate, hydrothermal approach, L-Dopa and sensor

PP-57

COST EFFECTIVE SYNTHESIS OF NICKEL TITANATE MODIFIED GLASSY CARBON ELECTRODE FOR THE DETECTION OF URIC ACID

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Abstract

The hydrothermally synthesized Nickel Titanate ($NiTiO_3$) was used for the electrochemical determination of Uric acid using $NiTiO_3$ modified GCE. Various Analytical techniques such as UV, FT-IR, XRD ,CV were confirmed the formation of Nickel Titanate. Subsequently the applicable electrochemical studies were applied and reported the considerable enhancement of electro catalytic activity of a Nickel Titanate. The proposed Nickel Titanate was developed as an electro catalyst for the sensitive determination of Uric acid. The electrochemical studies reveal that the Nickel Titanate has a good linear dependence and high sensitivity towards Uric acid. It also produces good practical availability. The proposed electrochemical sensor showed relatively 0.0141μM of LOD and higher sensitivity upto 1.496 μA μM^{-1} cm^{-2} were achieved.

Keywords: Nickel Titanate, hydrothermal approach, uric acid and sensor.

PP-58

HIGHLY SENSITIVE DETECTION OF LEVOFLOXACIN BY COPPER TUNGSTATE BASED NANOPARTICLE MODIFIED GLASSY CARBON ELECTRODE

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Abstract

In this study, Copper tungstate ($CuWO_4$) nanoparticles were synthesized using hydrothermal approach. The evolution of $CuWO_4$ nanoparticle was verified using FT-IR, UV and XRD analysis. Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS) and Differential Pulse Voltammetry (DPV) were the electrochemical characterization techniques implemented in this work. Levofloxacin, a quinolone antibiotic, was analysed using DPV method with super active wolframite structure of $CuWO_4$. The $CuWO_4$ modified electrode shows the higher oxidation peak current compared to bare GCE. Furthermore, levofloxacin revealed notable sensitivity of 40.76μA $\mu M^{-1}Cm^{-2}$ and low detection limit of 0.013 μM. $CuWO_4$/GCE electrode shows prominent selectivity, acceptable stability and high reproducibility.

Keywords: Copper Tungstate, Biosensor, Antibiotic and Levofloxacin.

PP-58

HIGHLY SENSITIVE DETECTION OF LEVOFLOXACIN BY COPPER TUNGSTATE BASED NANOPARTICLE MODIFIED GLASSY CARBON ELECTRODE

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Abstract

In this study, Copper tungstate ($CuWO_4$) nanoparticles were synthesized using hydrothermal approach. The evolution of $CuWO_4$ nanoparticle was verified using FT-IR, UV and XRD analysis. Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS) and Differential Pulse Voltammetry (DPV) were the electrochemical characterization techniques implemented in this work. Levofloxacin, a quinolone antibiotic, was analysed using DPV method with super active wolframite structure of $CuWO_4$. The $CuWO_4$ modified electrode shows the higher oxidation peak current compared to bare GCE. Furthermore, levofloxacin revealed notable sensitivity of 40.76µA $\mu M^{-1}Cm^{-2}$ and low detection limit of 0.013 µM. $CuWO_4$/GCE electrode shows prominent selectivity, acceptable stability and high reproducibility.

Keywords: Copper Tungstate, Biosensor, Antibiotic and Levofloxacin.

PP-59

ELECTROCHEMICAL DETERMINATION OF DOPAMINE USING ZINC COBALTITE MODIFIED GLASSY CARBON ELECTRODE

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Abstract

In this study, we developed the Zinc cobaltite ($ZnCo_2O_4$) using hydrothermal approach followed by calcination method. The $ZnCo_2O_4$ nanoparticle formation was confirmed using UV, FTIR and XRD analysis. The electrochemical characteristics were performed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV), and amperometric (i-t) technique. This nanoparticle has been utilized as an electrode modifier for the electro oxidation of Dopamine. Furthermore, it shows the enhancement in peak current and shift of the oxidation potential in a negative direction. This nature proves the better electrocatalytic activity of dopamine. Due to $ZnCo_2O_4$ higher surface area, it provides the low detection limit of 0.0847 µM and higher sensitivity 17.05 µA μM^{-1} Cm^{-2}. $ZnCo_2O_4$/GCE electrode shows prominent selectivity, acceptable stability and high reproducibility.

Keywords: Zinc cobaltite, Biosensor, Antagonist Drug and Dopamine

PP-60

HYDROTHERMAL SYNTHESIS OF BARIUM STANNATE MODIFIED GCE FOR ULTRASENSITIVE DETECTION OF 4-NITROANILINE

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Abstract

In this study, the Barium Stannate ($BaSnO_3$) was synthesized using facile hydrothermal method. Several Analytical techniques such as UV, FT-IR, XRD were analyzed and confirmed the formation of Barium Stannate. The cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), Differential pulse voltammetry (DPV), and Amperometric (i-t) technique were the electrochemical characterization studies accomplished in this work. The proposed Barium Stannate was developed as an electro catalyst for the sensitive determination of 4-Nitroaniline. Using the electrochemical approach towards the 4-Nitroaniline, reveals that the Barium Stannate has a better catalytic reaction with a transfer of two electrons and shows good linear dependence and high sensitivity. It also creates great practical availability. The proposed electrochemical sensor showed relatively 0.085 μ M of LOD and higher sensitivity of 36.6 $\mu A\ \mu M^{-1}\ cm^{-2}$. Hence it is proven that Barium Stannate /GCE is a cost effective, highly sensitive electrochemical sensor for the detection of 4-Nitroaniline.

Keywords: Barium Stannate, hydrothermal approach, 4-Nitroaniline and sensor.

PP-61

FACILE SYNTHESIS OF MANGANESE VANADATE FOR ELECTROCHEMICAL DETERMINATION OF VANILLIN

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Abstract

We developed a manganese vanadate (MnV_2O_6) via easy synthetic approach of hydrothermal followed by calcination method. The arrangement of manganese vanadate (MnV_2O_6) was determined by using various instrumentation methods like UV, FT-IR and XRD analysis. The characteristics study of cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV) and amperometric (i-t) techniques were electrochemically performed. For the sensitive and selective detection of vanillin, MnV_2O_6 was used as an electrode modifier. This study shows the enhancement of peak current and shift of the oxidation potential towards a negative direction than bare GCE. The fabricated electrode exhibited a low detection limit of 4.433 nM, sensitivity of 204.95 μ A μ M^{-1} cm^{-2}, and produces better selectivity and stability. The optimized sensor was successfully applied to detect vanillin in real samples, including ice cream, chocolate, and water, and their obtained recovery was 98.46–99.80%.

Keywords: Manganese vanadate, hydrothermal approach, vanillin and sensor.

PP-62

IN-SITU DECORATION OF $CuMn_2O_4$ (DELAFOSSITE) ON N DOPED CARBON SPHERE FOR OER APPLICATION

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Abstract

In the current situation, an inexpensive and effective electrocatalyst is crucial to overcome the slow kinetics of the anodic oxygen evolution reaction in fuel cells. One excellent attempt to speed up the complex and slow anodic reaction is the heteroatom doped in hollow mesoporous carbon sphere. The large-scale production of metal–air batteries, an appealing solution for next-generation energy storage, requires low-cost, earth-abundant. N doped $CuMn_2O_4$ delafossite powder composed of earth-abundant elements was synthesized by using Dopamine hydrochloride, Copper acetate tetrahydrate and Manganese acetate tetrahydrate. N-doped $CuMn_2O_4$ delafossite having the high conductivity, large active surface area, and increase in the number of catalytic sites induced by Cu doping (i.e., Cu^{2+} and Cu-N) can be beneficial to the overall electrocatalytic activities. Thus, low-cost, widely-available hollow mesoporous carbon spheres with heteroatom doping can be utilised in place of expensive catalysts used in fuel cells to circumvent the relatively slow kinetics of the anodic OER. The oxygen evolution reaction (OER) are considered essential for understanding the limitations of water splitting. In electrochemical studies for this work using three electrode system .This

material is characterized by powder X-ray diffraction, FT-IR, and Raman spectroscopy. More importantly, their electrocatalytic performances for oxygen evolution reaction (OER) have been fully investigated by linear sweep voltammetry. Their stability was also studied for cost-effective and active electrode material. Overall, our study demonstrated that $CuMn_2O_4$ delafossite possesses effective OER activity.

PP-63

STUDIES ON CHITOSAN/SERICIN BASED COMPOSITE FILM FOR ENHANCING ANTIBACTERIAL AND ANTIBIOFILM ACTIVITY FOR BIOLOGICAL APPLICATION

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Abstract:

This research focused on the fabrication of composite film with controlled drug release properties to control inflammation. Chitosan and Silk Fibroin were used as base polymers and crosslinked with diclofenac to form composite films by solution casting technique. Prepared hydrogels were analyzed by swelling analysis in deionized water and buffer solutions. Functional groups confirmation and development of new covalent and hydrogen bonds, thermal stability and crystallinity were evaluated by FTIR, TGA and XRD, respectively. Rheological properties including gel strength and yield stress, elasticity, porosity and hydrophilicity of prepared composite film were also evaluated. In vitro studies confirmed that prepared composite film have good biodegradability, excellent antimicrobial property and admirable cytotoxicity induced by the composite materials. Drug release profile along with the drug encapsulation efficiency of prepared composite film can release the drugs with desired temporal patterns of swelling kinetics mechanism followed fickian model. Bioplomer of chitosan has the limitation arise from the physical and chemical in stability as well as the high hydrophobicity which greatly restrict its functionality and efforts are made to overcome these drawbacks by blending of biodegradable polymer.

Keywords: Chitosan, Silk fibroin, Antibacterial, Anti-biofilm, Release behaviour.

PP-64

TOWARD ULTRASENSITIVE DETECTION: Cu@CQDs CATALYZED COLORIMETRIC ASSAY FOR H_2O_2 AND GLUCOSE

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Abstract

The study delineates a scientific inquiry involving Cu@carbon quantum dots (Cu@CQDs) synthesized via hydrothermal methods, elucidating their peroxidase-like attributes. Notably, these Cu@CQDs exhibited catalytic prowess, instigating the conversion of hydrogen peroxide (H2O2) and 3,3′,5,5′-tetramethylbenzidine (TMB) into oxidized TMB (ox-TMB) with an absorption peak at 652 nm. The investigation meticulously scrutinized the influence of environmental factors such as temperature, incubation duration, and acidity on the catalytic efficacy of Cu@CQDs. Through systematic optimization, pH 3.5, a temperature of 0 °C, a Cu@CQD volume of 300 µL, TMB concentration of 3.0 mM, and a 30-minute incubation period were identified as optimal conditions, yielding augmented absorbance at 652 nm. This optimization facilitated the precise quantification of H_2O_2 within the concentration range of 2.0–50.0 µM, with a notably low detection limit of 0.54 µM. Furthermore, acknowledging the relationship between H_2O_2 and glucose, a colorimetric methodology for glucose concentration determination was devised, underscoring the multifaceted utility of Cu@CQDs in analytical applications

Keywords: Cu@CQDs, Catalysis, H2O2, Glucose, Detection.

PP-65

OPTIMIZING ADDITIVES FOR BISMUTH MODIFIED ELECTRODES ON CARBON CLOTH: ENHANCING ELECTROCHEMICAL DETECTION OF Pb^{2+}

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Abstract

In this study, we focused on the development of environmentally friendly electrodes capable of detecting harmful substances like Pb^{2+}. Nano-crystalline Bismuth (Bi) electrodes were prepared through electrodeposition method, employing various additives such as methyl cellulose (MC) and polyvinylpyrrolidone (PVP), as well as without additives to effectively evaluate their impact when combined with methane sulfonic acid complexing agent. These Bi electrodes were deposited onto carbon cloth (CC) for sensing applications. We investigated and evaluated their quality and growth rate of deposited Bi films through XRD and FESEM techniques. Furthermore, we elucidated the stepwise fabrication process of the Bi-modified electrode and assessed their

electrochemical sensing capabilities towards Pb^{2+} in a neutral medium (pH 7.0) using differential pulse voltammetry (DPV) technique. Remarkably, the Bi-modified electrode demonstrated exceptional electrocatalytic activity for Pb^{2+} detection, suggesting its potential as an enhanced sensor for determining Pb^{2+} levels in water samples.

PP-66

OUTCOME OF PMMA FRONT SURFACE COATINGS ON mc-Si SOLAR CELLS BEFORE AND AFTER ENCAPSULATION

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Abstract

A new state-of-the-art encapsulation technique is needed for crystalline silicon device, in order to replicate its functionality on ground-based photovoltaics. In this context, we earlier demonstrated pouch lamination as a cost-effective and reproducible technique with better performance than a PMMA surface coated mc-Si cell. This work contains a comparative study of an unlaminated PMMA surface coated mc-Si solar cell with a laminated one. It is observed from the diffuse reflectance spectra that on laminating the PMMA coated cell, high energy photons are transmitted till 320 nm whereas visible and NIR photons are reflected on the

surface. Nevertheless, the charge generation is limited on lamination compared to the unlaminated PMMA coatings. This is evident in the electrical performance as well with 11.44% decrease in the short-circuit current of PMMA coated device which is already 0.05% lower than the bare and pouch laminated bare cells. Hence based on the optical and electrical behaviour, we suggest that the polymer thinfilm coatings could be efficient encapsulants that does not require a lamination component.

PP-67

ADVANCED 2D PHOSPHORENE-MXENE HETEROSTRUCTURES: A NOVEL APPROACH FOR HIGH-PERFORMANCE ASYMMETRIC SUPERCAPACITORS WITH EXTENDED OPERATING VOLTAGE RANGE

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Abstract

Nano-formulations utilizing two-dimensional (2D) inorganic phosphorene nanosheets have attracted considerable attention in the field of energy storage, specifically in the advancement of supercapacitors. Importantly, 2D materials provide slit-shaped ion diffusion channels that enable the rapid movement of ions greatly. Herein, we have effectively created an asymmetric device by utilizing conductive 2D Phosphorene/MXene (PMx) electrodes. The fabrication process utilized a two-step technique involving Liquid Phase Exfoliation followed by Ultrasonication. The confirmation of the layered structure of phosphorene on MXene nanosheets was achieved through the utilization of FE-SEM, HR-TEM, and AFM investigations. Further, XRD, EDX, and XPS techniques were used to confirm the structural integrity and chemical composition of the nanocomposites. The characterization studies revealed an essential understanding of how the distance between layers affects the electrochemical capabilities of 2D composite materials. The PMx electrode which was synthesized with a mass ratio of 2:1, showed a notable rate capability and retained 81.3% of its capacitance at a current density of 10 $A \cdot g^{-1}$. Furthermore, it demonstrated a durable cycle life and a substantial gravimetric capacitance of 310 $F \cdot g^{-1}$ at 1 $A \cdot g^{-1}$. The fabricated device also showed a remarkable energy density of 85 $Wh \cdot kg^{-1}$. This study provides insights into the development of next-generation portable, and highly integrated supercapacitors that have exceptional gravimetric and rate capabilities.

Keywords: Integrated supercapacitor; Energy density; 2D materials; Phosphorene; MXene.

PP-68

SYNERGISTIC POTENTIAL OF CHROMIUM (III) OXIDE/BOROPHENE NANOCOMPOSITE IN ENHANCING THE OPERATING VOLTAGE AND ENERGY DENSITY OF THE FABRICATED ASYMMETRIC SUPERCAPACITOR DEVICE

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Abstract

In today's world, clean energy storage devices, such as batteries, fuel cells, and electrochemical capacitors, have been recognized as one of the next-generation technologies to assist in overcoming the global energy crisis Herein, we have synthesized a sandwich-type nanocomposite comprising Cr_2O_3 nanoparticles and Borophene nanosheets via hydrothermal and ultrasonication method. The prepared Cr_2O_3-Borophene NCs structural, functional, morphological, and elemental analyses were investigated using XRD, FE-SEM, HR-TEM, and XPS analysis techniques. The obtained electrochemical results from the three-electrode set-up suggest that the fabricated Cr_2O_3-Borophene NCs can store charges via faradic and EDLC reactions. Subsequently, the Cyclic Voltammetry (CV) study revealed that the synthesized composite delivers a higher specific capacitance 943 Fg^{-1} at 10 mVs^{-1}. Whereas, Galvanostatic charge discharge (GCD) evaluation demonstrated that at 1 Ag^{-1} current density the nanocomposite material delivered 890 Fg^{-1} specific capacitance. GCD analysis also reveals good stability, redox rate capability, and faradaic nature of the nanocomposite coated on Ni-foam. The electrochemical impedance spectra (EIS) revealed lower solution resistance (R_s), and charge transfer resistance (R_{ct}) of 0.68 Ω and 1.43 Ω, respectively. The cyclic stability of the Cr_2O_3-Borophene NCs exhibited good capacitive retention of 83.7% even after 3000 continuous cycles.

Keywords: Energy Crisis; High power density; Cr_2O_3; Borophene; Supercapacitor.

PP-69

EXPLOITING $FeCl_3$ AS AN ACTIVATOR TO TRANSFORM BIOMASS INTO CARBON ELECTRODE MATERIAL FOR ENERGY STORAGE APPLICATIONS

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Abstract

Energy storage technologies with practical uses include batteries and supercapacitors. The poor performance of the electrode has impeded the development of these energy storage devices. Due to its low cost, ease of processing, and excellent stability, biomass from waste plants presents a promising green option for energy storage device electrodes. This work describes the research of using lotus seedpods (LS) as a biomass precursor in a two-step fabrication method to convert biomass into activated carbon electrode material with high electrical conductivity or low electrical resistivity. First, the LS is precarbonized and then subjected to simultaneous pyrolysis and activation with $FeCl_3$, resulting in LS-derived activated carbon material. The activated carbon material's structural and functional properties were analyzed using XRD, Raman, and FT-IR. The morphology and texture of carbon materials were examined using SEM and BET analysis. Activated porous carbon prepared in this study showed a BET surface area of 99.614 m^2/g and an average pore size of 3.52 nm. Based on these results, the electrode produced from this carbon material is expected to be an excellent electrode material for energy storage applications.

Keywords: Lotus seedpod, $FeCl_3$, Pyrolysis process, Electrode material, Energy storage devices.

PP-70

PHYTOCHEMICAL ANALYSIS AND ANTIBACTERIAL STUDIES OF ETHANOLIC LEAF EXTRACT OF *ACALYPHA INDICA* HERBAL PLANT

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Abstact

Acalyphaindica L. is one of herbal plants found in wet, moderate, tropical areas which grows as a weed. This herb has been used traditionally to treat dysentery, diarrhea, malnutrition, and malaria. But chemical compoundspresent inethanolic extract of leaves of*Acalyphaindica*L. hasn't been completely reported yet. The present study was extraction of pure compounds from leaf of Acalyphaindica using ethanol and investigate the phytochemicals presence and antibacterial activity against the Gram negative bacterial strains ofSalmonella typhi,Escherichia coli and Gram-positive bacterial strains of *Enterococcus faecalis*Bacillus cereus.

Key words: Acalyphaindica L, Ehanol, Phytochemicals, Antibactrial activity

PP-71

COPPER OXIDE NANOPARTICLES AND THEIR CHARACTERIZATION: SYNTHESIS USING GREEN SOLVENTS- TERNARY DEEP EUTECTIC SOLVENTS

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Abstract

Deep Eutectic Solvents were generated by combining hydrogen bond donors and halide salts that turn liquids at room temperature. Due to their similarities to ionic liquids, Deep Eutectic Solvents are now commonly recognized as a new class of ionic liquids. Due to the relatively inexpensive components and their straightforward synthesis, which produces little waste and doesn't call for additional purification procedures, they are frequently affordable. Using a more environmentally friendly process called the evaporation method, we developed three different kinds of ternary deep eutectic solvents, and physical properties such as pH, conductivity, density, viscosity, and fourier transform infrared spectroscopy were taken. The prepared ternary deep eutectic solvents were utilized as a medium for the chemical reduction process of synthesizing copper nanoparticles. By Visible spectroscopy, Fourier transform infrared spectroscopy, X-ray diffraction pattern, Scanning Electron Microscopy, and Energy

Dispersive x-ray analysis techniques, the synthesized copper nanoparticles were evaluated. Copper Visible spectroscopy, Fourier transform infrared spectroscopy, X-ray diffraction pattern, Scanning Electron Microscopy, and Energy Dispersive x-ray analysis techniques, the synthesized copper nanoparticles were evaluated. Copper nanoparticles were widely used in the nanomedicine field.

PP-72

CRYSTAL STRUCTURE AND COMPUTATIONAL STUDIES OF BIS(2-AMINO-1,3-BENZOTHIAZOLE−κN^3)DICHLORIDOZINC(II)

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Abstract

To explore the crystal structure of Bis(2-amino-1,3benzothiazole-κN^3)dichloridozinc(II). The structure of the title compound was confirmed by single crystal X-ray diffraction studies. The SC-XRD study revealed that the crystal is in monoclinic system with space group P 21/C1 and the lattice parameters a = 11.7330(5)Å, b = 7.3680(3)Å, c = 17.5388(9) Å ($\alpha = 90°, \beta = 10°, \gamma = 90°$). The Zn^{II} atom is coordinated by two nitrogen atoms of 2-aminobenzothiazole ligand and two chlorine atoms within a distorted tetrahedral geometry. The molecular structure is stabilised by intramolecular N-H…Cl hydrogen bonds. DFT calculations were done by utilizing basis set (DFT/B3LYP/6-311G++(d,p)). In addition, 2D- finger print plot was employed to determine the intermolecular interactions and the crystal packing by using Crystal explorer 21.5.

Keywords Single crystal XRD, Tetrahedral, 2D-finger print plot.

PP-73

MoO_3/SiO_2/GRAPHENE NANOCOMPOSITE AS EFFECTIVE ELECTROCHEMICAL SENSING PLATFORM FOR VANILLIN

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Abstract

Vanillin is the primary fragrance component in vanilla. Dried vanilla pods contain up to 2% vanillin. Vanillin can be used as a coloring additive on thin-layer chromatography plates to monitor chemical reactions. However, vanillin can trigger allergic responses and worsen migraine symptoms. According to the United Nations Food and Agriculture Organization, daily vanillin consumption should not exceed 10 mg/kg. Therefore, determining vanillin in food is crucial. Molybdenum oxide (MoO_3)-based nanomaterials have excellent catalytic performance in a variety of electrochemical sensing applications, as well as enhanced catalytic and electrochemical characteristics. Novel electrocatalyst technologies and their application to food additive monitoring are of great interest. In this study, we used the hydrothermal technique to create a MoO_3/SiO_2 nanocomposite. While the graphitic carbon nitride sheets were incorporated into the MoO_3/SiO_2 and tested its electrochemical sensing capability for vanillin detection. The improved sensor achieved large linear ranges low limit of detection (LOD, 60 nM) by differential pulse voltammetry (DPV). Furthermore, the practical application of the proposed sensor was successfully tested in food samples, with an outstanding recovery rate.

Keywords: gC_3N_4, MoO_3/SiO_2, electrochemical sensing, vanillin, DPV

PP-74

LEAD-LIKENESS SCRUTINIZATION OF PYRROLES

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Abstract

Pyrroles are widely recognized as biologically active scaffold possessing diverse nature of activities and featuring different pharmacophores in a pyrrole ring system leading to the formation of more active compounds. Pyrrole scaffold has been incorporated into many active drugs acting as anticancer, anti-hyperlipidemic, anti-inflammatory, and anti-fungal agents. The pyrrole ring is also a reactive scaffold for polymerization, inhibiting corrosion, solvent for resins, and intermediate in organic synthetic reactions. Physicochemical, pharmacokinetics, drug like and related parameters of the subjected pyrrole molecule can be derived from the web based tool, SwissADME, a free open access and fast predictive models showing its significance, predictive power, intuitive interpretation and straight forward translation to molecular design. SwissADME is an user friendly graphical interface for the cost and login-free website, enable easy input and efficient analysis of the output which does not require any prior knowledge in Computer Aided Drug Design (CADD). From the results obtained through SwissADME of subjected pyrrole derivatives, we have evidenced that most of the pyrrole derivatives were found to possess drug-likeness properties. Form this study, the ADME property of the pyrrole derivatives is disclosed for researches, which can be used further identification of their *in vitro* and *in vivo* therapeutic potentials. SwissADME's strong points are non-exhaustively different input methods, computation for multiple molecules, and the possibility to display, save and share results per individual molecule or through global intuitive and interactive graphs.

PP-75

RHODAMINE BASED FLUORESCENT PROBES FOR DETECTION OF HYDROGEN PEROXIDE IN AQUEOUS MEDIUM AND LIVE CELL IMAGING

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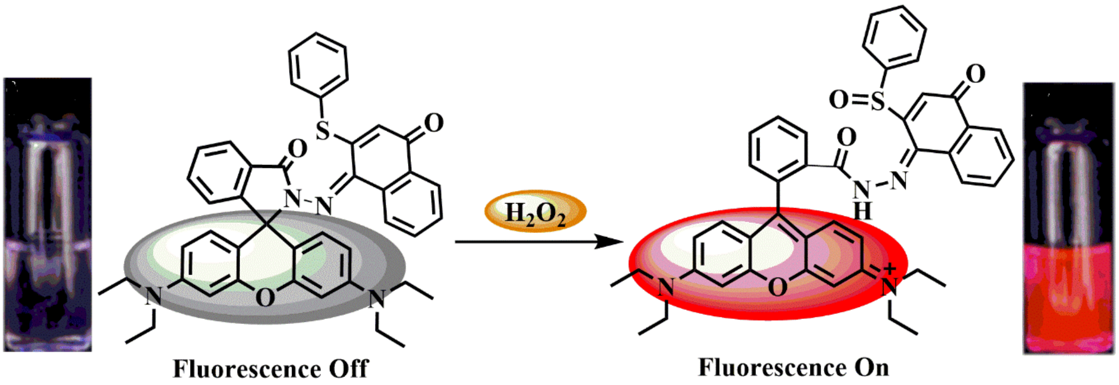
Abstract

The dye RS1 based on rhodamine was prepared as new fluorescent probes for hydrogen peroxide (H_2O_2) detection in live cells imaging. The dye RS1 was characterized using NMR spectroscopy, UV-visible, emission spectroscopy and mass spectrometry. The fluorescent dye RS1 has fluorescence maximum at 580 nm and the colour changes from colourless to red in visual naked eye detection on the addition of H_2O_2. The fluorescence intensity of the reaction between hydrogen peroxide and dye RS1 is linear in the hypochlorous acid concentration range of 0 to 100 µM with a detection limit of 40 nM in fluorescent spectrometry method. The sensing is further supported by the ^{1}H NMR titrations which reveal that the reactive oxygen species of H_2O_2 bind to the -S- unit of RS1. The Chemosensor also showed excellent performance when used in the “test strip” method.



Scheme 1. Sulphur-containing rhodamine-based fluorophore **RS1**

PP-76

ROOM-TEMPERATURE H_2S GAS SENSORS USING PEROVSKITE-TYPE $SrSnO_3$ ADORNED WITH A REDUCED GRAPHENE OXIDE NANOCOMPOSITE

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Abstract

2D carbon structure /Metal oxide nanocomposites have received great attention in various fields of science and technology, especially for developing high-performance gas sensors. In the present article, we demonstrate in detail the facile synthesis of rGO perovskite $SrSnO_3$ nanocomposite and its selective Hydrogen Sulfide (H_2S) sensing behaviour. The synthesized materials were characterized by analytical and morphological techniques such as X-ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM), and High Resolution-Transmission Electron Microscopy (HR-TEM). $SrSnO_3$ exhibits nanoballs-like morphology due to the self-assembly of smaller nanoparticles into hierarchical structures and decorated over the rGO sheet. The e-waste circuit board (e-WCB) modified rGO-$SrSnO_3$ nanocomposite chips towards the 10-ppm H_2S produce a maximum sensitivity of 61 % with the appreciable fast response of (12 s) and recovery time (11 s) at room temperature and the sensor exhibits excellent sensitivity of 72 % at higher concentration (100 ppm) of ammonia. Furthermore, the sensor was highly active and selective towards H_2S compared to other interfering gases. As a consequence, the $SrSnO_3$ decorated rGO nanocomposite is a promising candidate for quick, sensitive, and selective detection of H_2S at room temperature (30 °C).

Keywords: perovskite, $SrSnO_3$, rGO_4, nanoballs, ammonia, and gas sensor.

PP-77

ENHANCED ELECTROCHEMICAL PERFORMANCES OF LIMN$_2$O$_4$ CATHODE MATERIALS BY COATING WITH AlPO$_4$ NANOPARTICLES

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Abstract

One of the challenges for improving the performance of lithium ion batteries to meet increasingly demand requirements for energy storage is the development of suitable cathode materials. Aluminium phosphate coated to the surface of the spinel $LiMn_2O_4$ powder material was prepared by a sol–gel method and subsequent heat treatment at 600 ºC for 8 h. Surface modified $LiMn_2O_4$ materials were characterized by using TG/DTA, X-ray diffraction, Scanning electron microscope, X-ray photoelectron spectroscope, cyclic voltammetry techniques and charge/discharge studies. X-ray diffraction results illustrate that no significant bulk structural differences are observed between the $AlPO_4$ coated $LiMn_2O_4$ and uncoated

$LiMn_2O_4$. TEM results indicates that, the $AlPO_4$ was completely coated over the surface of the $LiMn_2O_4$ core materials and also this results confirmed by XPS analysis. Galvanostatic charge/discharge studies of the uncoated $LiMn_2O_4$ and $AlPO_4$ coated $LiMn_2O_4$ cathode materials were carried out in the voltage range between 3.0 and 4.5 V. The composition of $AlPO_4$ coating was increased from 0.0 to 3.0 Wt.%, the initial capacity of the samples decreased slightly. Moreover the cycling stability was increased remarkably between 3 - 4.5 V. 2.0 Wt.% $AlPO_4$-coated $LiMn_2O_4$ cathode has satisfied the structural stability, high reversible capacity and excellent electrochemical performances. Surface modification treatment should be an effective way to improve the comprehensive properties of the cathode materials for lithium ion batteries.

Key words: $AlPO_4$-coated $LiMn_2O_4$, XRD, XPS, Charge/discharge

PP-78

SYNTHESIS, SPECTRAL CHARACTERIZATION OF 3-(2,3-DICHLOROSTYRYL)-5,5-DIMETHYLCYCLOHEX-2-ENONE. A COMPREHENSIVE EXPERIMENTAL, COMPUTATIONAL, DOCKING METHODS AND ADME PROPERTIES.

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Abstract

The compound 3-(2,3-dichlorostyryl)-5,5-dimethylcyclohex-2-enone was synthesized by Claisen Schmidt condensation and characterized by different spectral studies. Furthermore, the chemical structure of the title compound was ascertained by spectral techniques including FT-IR, ^1H, and ^{13}C NMR spectroscopy. ***The synthesized compound was compared with the***

experimental values to the computational values by utilizing 6-31G (d, p) as the basis set, Calculations have been made to determine the electrical dipole moment (μ) and initial hyperpolarizability (βo). The estimated outcome (βo) indicates that the chemical in the title may exhibit nonlinear optical (NLO) activity. Calculations were made of the molecular electrostatic potential (MEP) and the Mulliken charges. The HOMO-LUMO energies were determined, and natural bonding orbitals (NBO) were examined. Molecular docking studies of the synthesised compound were performed in the auto dock using the different proteins and it proved that the synthesized compound exhibit good binding affinity. In addition to that, the physiochemical and pharmacokinetic features of the compound were analysed using the Swiss ADME online application.

Keywords: Claisen Schmidt condensation, Spectroscopic studies, DFT calculations, Molecular docking, Insilco ADMET.

PP-79

DESIGN OF PLASMONIC METALLIC SILVER-INDUCED ZNO NANOSTRUCTURE FOR IMPROVED PHOTOCATALYTIC DEGRADATION AND ELECTROCHEMICAL ACTIVITY

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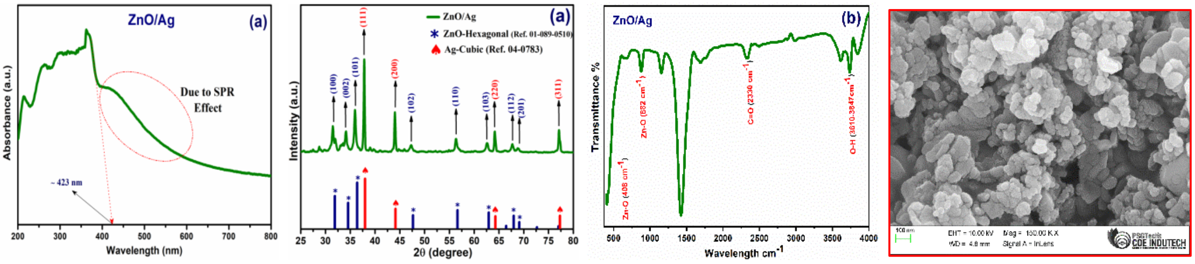
Abstract

A one-step microwave irradiation method was used to create a hybrid nanocomposite of ZnO and plasmonic silver. Characterization of the composite was conducted using various



techniques, such as XRD, SEM, UV-Vis DRS, PL, and FT-IR spectroscopy to evaluate its structural, morphological, optical, electrical properties, and chemical bonding. The XRD pattern confirmed the purity and formation of ZnO-Ag plasmonic hybrids with ZnO exhibiting a hexagonal wurtzite crystal phase and Ag nanoparticles displaying a face-centered cubic structure. The photocatalytic performance of the hybrids was evaluated by measuring the degradation percentage of different dyes under visible light irradiation. Results showed high degradation percentages for various dyes. The electrochemical studies revealed that the ZnO-Ag catalyst produced a current density of 14.72 mA/cm^2 for the oxygen evolution reaction and 23.68 mA/cm^2 for the hydrogen evolution reaction. The high photocatalytic efficiency was attributed to the enhanced photoabsorption ability and reduced recombination rate resulting from the formation of ZnO-Ag heterojunction, which was further amplified by the surface plasmon resonance effect from the Ag nanoparticles. This study demonstrates the potential of ZnO-Ag plasmonic hybrids for dye photocatalytic degradation and energy production applications.

Keywords: Ag anchored ZnO · Nanohybrid · Surface Plasmon Resonance · Photocatalyst · Electrocatalyst

PP-80

INCLUSION COMPLEX DERIVED CARBON MATERIAL AS A NEGATIVE ELECTRODE MATERIAL FOR SUPERCAPACITOR APPLICATIONS

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Abstract

In today’s world utilization of energy increases with rapid growth of population but storing a huge amount of energy is a competitive one. Energy storage involves in converting one form of energy into another which can be utilized later. Supercapacitor (SC) is one of the promising systems which comes under electrical energy storage devices. Inclusion complex is defined as host-guest chemistry where host has a cavity and guest gets accommodated into it. In this work, the inclusion complex is prepared from β-Cyclodextrin (β-CD) has hydrophobic inner cavity which plays host role, guest molecules are anthraquinone (AQ) and 1-aminoanthraquinone (N-AQ) which contains oxygen and nitrogen as heteroatoms respectively. Then, the complexes are involving carbonization processes and produce the activated carbons (ACs). The materials are characterized by SEM, TEM, XRD, RAMAN and EDX. The prepared carbon materials electrochemical performance is studied using Cyclic voltammetry (CV) and Galvanostatic charge-discharge studies. The nitrogen doped carbon shows higher specific capacitance value of 854 Fg^{-1} at current density of 1 Ag^{-1}. This result suggested that the nitrogen doped carbon is a promising material for SC applications.

Keywords: Energy storage, Supercapacitor, EDLC, Inclusion complexes.

PP-81

ASYMMETRICALLY FUNCTIONALIZED ACCEPTOR END-CAPPED TRIARYLAMINES FOR HIGH-PERFORMANCE NON-VOLATILE RESISTIVE MEMORY DEVICES

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Abstract

Organic-based resistive memory devices have emerged as promising candidates for next-generation information storage applications, providing new possibilities for realizing high-performance organic electronics. Herein, we have designed and synthesized a triphenylamine-based donor-acceptor (D-A) system with varying acceptors such as nitrophenyl, cyanophenyl, trifluoromethylphenyl, and

formyl phenyl units. The photophysical studies reveal an absorption maximum of 235-345 nm, which ensures better charge transfer between the donor and the acceptor unit. The electrochemical analysis showed an irreversible anodic peak in the 1.07-1.08 V range, ensuring the triphenylamine unit's one-electron oxidation. All the fabricated devices exhibited non-volatile write-once-read-many (WORM) memory behavior. The compounds substituted with trifluoromethylphenyl unit showed a maximum current ON/OFF ratio of 10^3 with a threshold voltage of 2.05V, and the compound with cyanophenyl substituent showed a current ON/OFF ratio of 10^2 at a threshold voltage of 2.7 V. The device stability was measured by retention and endurance characteristics up to 1000 s and 100 cycles. The molecular simulations were analyzed using Density Functional Theory (DFT) calculations, which confirms the possible mechanism for the memory behavior. These studies reveal that substituting different acceptors in the D-A architecture could improve memory performance.

PP-82

DESIGN AND SYNTHESIS OF SOLUTION-PROCESSABLE FUNCTIONALIZED ANTHRACENES FOR BISTABLE RESISTIVE MEMORY DEVICE APPLICATIONS

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Abstract

Organic resistive memory devices represent a promising frontier in electronics, offering efficient and versatile solutions for next-generation data storage and computing applications. Here, we have designed and synthesized a series of donor-acceptor (D-A) based anthracene compounds for non-volatile memory devices. The D-A architectured compounds were synthesized using anthracene donor and various acceptor units through Suzuki-Miyaura coupling reactions to get a binary write-once-read-many (WORM) memory behavior. The

optical investigations revealed an absorption maximum of around 485 nm in trifluoromethylphenyl substituted anthracene, which is attributed to the intramolecular charge transfer between the donor and the acceptor moiety. Besides, the electrochemical studies exhibited an irreversible anodic peak in the range of (0.9 – 1.1V), indicating the oxidation of the anthracene unit. All the fabricated devices showed binary Write-Once-Read-Many-Times (WORM) memory characteristics. The compounds substituted with fluorophenyl onto the anthracene core showed a current ON/OFF ratio of 10^4 with a low threshold voltage of -1.83 V. The stability of the devices was measured with retention and endurance characteristics up to 10^3 s and 100 cycles. This study provides a new vision of the influence of terminal acceptors in D-A architecture on the performance of organic small molecule-based resistive memory devices.

PP-83

SYNTHESIS AND CHARACTERIZATION OF PICRORHIZA ROOT EXTRACT DERIVED SILVER NANOPARTICLES

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Abstract

The green synthesis approach has garnered interest in the synthesis of nanoparticles due to its simple process, economical nature, and environmental friendliness. Generally, green synthesis techniques are used to produce metal, metal oxide, and carbon nanoparticles. Among them, the use of silver nanoparticles (AgNPs) in biological sensors, plasmonics, optoelectronics, catalysis, and antibacterial properties is rapidly increasing[1]. It has various characteristics, such as a high surface to volume ratio and unusual size and shape. biological

characteristics and strong electrical conductivity[2]. Here, we synthesized AgNPs utilizing Picrorhiza root extract without the need of a reducing agent. FT-IR, XRD, HR-TEM, and UV-visible spectroscopic methods provided excellent characterizations of the produced AgNPs. The produced nanoparticles exhibit an SPR band at 413 nm and are persistent for several months (Figure 1A). The estimated size of the particles is 16 ± 0.5 nm (Figure 1B). In the future, we will use these silver nanoparticles for research on their antibacterial properties[3].

PP-84

SOLUBILITY ENHANCEMENT OF DRUG LOMUSTINE USING BETA-CYCLODEXTRIN INCLUSION COMPLEXES

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Abstract

Lomustine has very low water solubility. It forms a complex with beta-cyclodextrin (beta-CD) both in aqueous and in solid state. It was observed that due to formation of the inclusion complex, the solubility and dissolution rate of Lomustine were enhanced. The formation of 1:1 complex with beta CD in solution was confirmed by phase solubility and spectral shift studies. The solid inclusion complexes of Lomustine and betaCD were prepared by the kneading method using different molar proportions of betaCD, and formation of solid inclusion complexes of Lomustine and betaCD at different molar ratios were confirmed by differential scanning calorimetry. Enhancement of dissolution rates with increasing quantity of betaCD in the complex was observed. It was also observed that the complexes exhibit higher dissolution rates than the pure drug and physical mixture.

Keywords: Lomustine, Betacyclodextrin, Dissolution, Kneading Method

PP-85

BIOTEMPLATE-ZnO/GRAPHENE NANOCOMPOSITE FOR BETTER THERMAL AND PHOTOCATALYTIC DEGRADATION

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Abstract

Biotemplate-ZnO/graphene nanocomposite synthesized by hydrothermal method using chitosan as a biosurfactant, graphene, zinc chloride as a source materials and sodium hydroxide as precipitating agent. The functional groups of resultant matrixes from chitosan, ZnO and graphene were characterized and confirmed by FTIR and RAMAN Spectroscopy. The crystallite size of the nanocomposite was confirmed by XRD. Surface morphology of the synthesized nanocomposites was analyzed by HR-SEM with EDAX and TEM analysis. The chitosan-ZnO particle intercalated graphene layer, thermal stability was analyzed by TG-DTA; the results demonstrate that chitosan-ZnO intercalated graphene has reinforced effect compared to among the components. Furthermore, the biotemplate-ZnO/graphene nanocomposite for better photocatalytic degradation than composite. Therefore, Biotemplate connected on ZnO intercalated to graphene can be promising materials for photocatalytic degradation applications.

Key words: Chitosan-ZnO, graphene, nanocomposite, thermal stability, Photocatalytic degradation

PP-86

NANO-STRUCTURED SPHERICAL CHITOSAN-SnO_2/PVP COMPOSITE FOR BETTER THERMAL AND PHOTOCATALYTIC PERFORMANCE

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Abstract

A new Chitosan based SnO_2 intercalated PVP matrix was successfully synthesized by hydrothermal route. The chemical bonding of chitosan, PVP and O-Sn-O functional groups were confirmed by FT-IR analysis. XRD patterns confirm the semicrystalline nature and the incorporation of Sn^{4+} ions into PVP matrix. The chitosan-SnO_2 sphere like structure particles are covered with capping agent of PVP in the nanometer level analyzed from HR-SEM and TEM analysis. Thermal stability of cationic biopolymer based SnO_2 intercalated PVP was higher than chitosan-PVP and chitosan. The results demonstrate that chitosan-SnO_2 intercalated PVP matrix has synergistic effect compared to chitosan-PVP. Therefore, biopolymer based SnO_2 intercalated to PVP matrix act as a better photocatalytic performance of methylene blue dye under sunlight irradiation. The CSP appear to be the new promising material in dye removal application with 90.2 %, regeneration after four cycles.

Key words: Chitosan-SnO_2, PVP, Sphere structure, Thermal stability, Photocatalytic performance.

PP-87

SYNTHESIS, SPECTRAL CHARACTERIZATION AND ANTIBACTERIAL STUDIES OF 2-AMINO-ISOINDOLE-1,3-DIONE – INSILICO MOLECULAR DOCKING, ADMET AND DFT STUDIES

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Abstract

The newly synthesised 2-amino-isoindoline-1,3-dione is characterized by IR, ^{1}H NMR and ^{13}C NMR spectral analysis. The physicochemical and pharmacokinetics feature of the compound is studied using online Swiss ADME application. The Compound showed good activity towards antibacterial compared with standard. The compound carried out molecular docking using Auto-dock and shows appreciable binding affinity against 6W63 protein. The energy gap (E_g), frontier orbital energies (E_{HOMO}, E_{LUMO}) and reactive parameters like chemical hardness and global hardness and Mulliken charges are calculated using Density functional theory.

Keywords: Isoindole, Docking, ADMET, Antibacterial and DFT

PP-88

SYNTHESIS OF Nd DOPED TiO₂ NANOMATERIAL FOR DYE SENSITIZED SOLAR CELLS AND PHOTOCATALYTIC APPLICATIONS

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Abstract

The rapid growth in the global population has led to higher energy consumption and environmental pollution. One of the serious environmental pollution is water pollution caused by dyes from the industries like textiles, paint and food processing units. There has been a growing focus on creating new environmental friendly technologies to conserve the energy and protect the environment for future generation. With depleting non-renewable energy, the renewable solar energy has gained wide attention in the research circle. Currently, novel nanomaterials are being developed to provide shorter reaction pathway with enhanced properties. The present work deals with the synthesis of Nd doped TiO_2 nanomaterial by sol-gel method. The obtained sample is characterized by XRD, EDAX, SEM and UV-DRS. Modification of TiO_2 by Neodymium was found to enhance its properties. The synthesized material was used as a photoanode for DSSC, in which 0.6 % Nd-TiO_2 provide higher power cconversion efficiency of 3.75 %. The photocatalytic application of 0.6 % Nd-TiO_2 exhibited 93 % degradation efficiency for Rhodamine B dye under visible light.

PP-89

S-DOPED g-C_3N_4 /FeCo-LDH HETEROSTRUCTURED PHOTOCATALYST FOR EFFICIENT HYDROGEN PRODUCTION IN VISIBLE LIGHT

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Abstract

In the realm of renewable energy technologies, the development of efficient photocatalysts for hydrogen production holds paramount importance. The photocatalytic activity from a single semiconductor suffers from inherent limitations such as rapid recombination rate, ineffective utilization of photogenerated charge carries, photocorrosion, and stability of the photocatalyst. Here, we demonstrate a heterostructured semiconductors to mitigate the inherent limitation of a single semiconductor. Graphitic carbon nitride (g-C_3N_4) is a promising and visible active candidate that has created much attention in the area of photocatalyst due to its unique band edges that cover both hydrogen and oxygen evolution potential, and high chemical and thermal stability [1]. To improve the H_2 production efficiency in visible light, heteroatom doping in g-C_3N_4 and heterostructure formation with FeCo-LDH have been carried out. The FeCo-LDH with a band gap of 2.1 eV that covers hydrogen evolution potential led to a notable enhancement in the H_2 generation rate of 5025 μmol/h/g_{cat} which is 28 times higher activity compared to pristine g-C_3N_4 [2]. This work elucidates that the exceptional conductivity of FeCo-LDH expedites the transfer of photogenerated electrons from S-doped g-C_3N_4 to the conduction band of FeCo-LDH.

Keywords: Photocatalyst, g-C_3N_4, Heterostructure, Doping, Hydrogen Evolution.

PP-90

AN OPTICAL PROPERTIES OF ALPHA MANGANESE OXIDE THIN FILMS SYNTHESIZED USING SPIN COATING TECHNIQUE

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Abstract

In this present work, the α-MnO_2 thin film was prepared on a glass substrate via sol-gel

spin-coating technique. The prepared thin film was poked in air atmosphere at 450ºC for 1hour. The obtained α-MnO_2 thin film has been subjected to analyze the structural, particle size, optical property with band gap, functional group analysis and crystallite defects using the X-ray diffraction (XRD), UV-Vis Spectrophotometer (UV), Photoluminescence (PL) and Raman Spectrometry respectively. The X-ray diffraction analysis confirmed the formation of α-MnO_2 with tetragonal structure (JCPDS No.:72-1982). The band gap of the prepared film was determined using UV-Vis absorption spectral data followed by Tauc's plot method to be 1.58 eV. The Raman spectrum of the MnO_2 thin film exhibited two prominent bands at 580 and 642 cm^{-1}, these bands correspond to lattice vibrations of Mn-O in MnO_2 and stretching vibrations of Mn-O in MnO_6, respectively. The PL spectra revealed two different emission peaks at 362 and 439 nm it is due to an existence of ultraviolet emission band at 362 nm and additionally a strong blue emission peak at 439 nm resulted from oxygen vacancy-related defects present in the prepared film.

PP-91

A NOVEL FLUORESCENT CHEMOSENSOR FOR Al^{3+} ION BASED ON SCHIFF BASE DERIVATIVE IN AQUEOUS SOLUTION

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Abstract

In acidic soils, aluminium is present in its solubilized form, Al^{3+}, which is poisonous to both plants and animals. Al^{3+} detection and measurement are essential for biology as well as chemistry. A novel Schiff base (SB) has been synthesized and the interaction of SB with different metal ions has been studied using fluorescence spectra. The results show that SB is a highly selective and sensitive probe for Al^{3+} ions over other commonly coexisting metal ions

in aqueous medium. A very obvious fluorescence enhancement effect was observed, and a turn-on ratio over 100000- fold was triggered with the addition of 10 equiv. of Al^{3+} ions. The complex solution (SB–Al^{3+}) exhibited reversibility with EDTA. These results may be caused by the formation of chelating ring structure with metal ion.

Keywords: Schiff base, Fluorescent chemosensor, Al^{3+} Chemosensor

PP-92

ECOFRIENDLY ULTRASONIC NATURAL DYEING OF WOOL FABRIC WITH NATURAL DYES OBTAINED FROM *WRIGHTIA TINCTORIA*

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Abstract

Natural dyes are extracted from plants, insects and minerals. Certain limitations of the natural dyes, they were withdrawn with the invention of synthetic dyes. In the long run, synthetic dyes were found to be harmful to the chemicals. As a result natural dyes have come to be used for their many intrinsic values. The main reason being, then availability of local plants as the main source of natural colorants. Almost all the parts of the plants, namely stem, leaves, fruits, seeds, barks etc are used for extracting natural colour. In addition, they are antimicrobial antifungal, insect repellant deodorant, disinfectant and they also have medicinal values. The present study was conducted to evaluate the colouring component and extraction method of plant dyes. Leaves of the plant are the source of dye. This dye was used to dye wool

by applying different mordanting methods with different mordant. Their easy availability in the country being zero cost effective and planted for other purposes are the main reasons for utilizing them as natural dyes.

Keywords: Ultrasonic dyeing; Natural dye; *Wrightia tinctoria*; wool

PP-93

ANTIFUNGAL STUDIES OF COBALT NANOPARTICLES USING NATURAL PLANT EXTRACT AND THEIR CHARACTERIZATION BY GREENER WAY

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Abstract

The development of sustainable green chemistry methods for manufacturing of metal nanoparticles has become prominence in recent years. They have investigated environmentally sustainable approaches for producing well-characterized nanoparticles. The use of living things to produce metal nanoparticles is one of the most widely explored techniques. Plants appear to be the best options among these creatures and are suited for the large-scale production of nanoparticles. Significant concentrations of several important phytochemicals, including vitamins, phenols, alkaloids, terpenoids and tannins are found in plant extracts. These phytochemicals function as catalysts for the reduction, capping, and stabilization of metal nanoparticles from their corresponding precursors. Cobalt nanoparticles are created when A. lanata extract is utilized as a reducing and stabilizing agent. UV-Visible Spectroscopy, FTIR spectra, XRD, and SEM with EDX microscopic analysis were used to analyze the produced cobalt nanoparticles. Researchers are paying close attention to cobalt nanoparticles due to its unique uses in a variety of fields, including photocatalysis, antimicrobial activity, and electrochemical sensing. Cobalt nanoparticles showed extremely powerful antifungal activity

in tests against harmful two fungal strains.

Keywords: Biomethod, Co NPs, UV-Visible, FTIR, XRD, SEM and Antifungal.

PP-94

A CHEMICAL ANALYSIS STUDY OF DRINKING WATER FROM SIVAGANGAI DISTRICT, TAMILNADU, INDIA

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Abstract

Individuals depend on the bottled water's quality, believing it to be free of health risks and microbiological contamination. The purpose of this study was to measure the levels of trace metal ions and certain physiochemical characteristics in drinking water samples from nearby villages in the Tamilnadu region's Shivagangai area, where the water is not treated before use. Determining the water quality from various sources was the goal. Ten sampling stations provided samples, which were then examined for the following characteristics. . Each sample was analysis for, Fe, Cu, Mn, Zn, Al, NO^{3-} , $SO4^{\ 2-}$, and F- using procedures outline in the Palintest Photometer Method (Palintest Photometer 5000) for the examination of water and waste water. The following parameters were measured: Contamination, Fe, Cu, Mn, Zn, pH, calcium, nitrate, electrical conductivity, and total dissolved solid. Average temperature, pH, total aerobic and anaerobic count, electrical conductivity, total dissolved solids and total hardness values are 13.6 ^{o}C, 7.4, 1.143 S/m, 571.67 mg/l and 362.67 mg/l in $CaCO_3$ respectively. The result shows that, except the total hardness and electrical conductivity all the parameters fulfill the minimum and maximum permissible limit for drinking water guidelines. However, it is also important to investigate other potential water contaminations such as chemicals and microbial and radiological materials for a longer period of time, including

human body fluids, in order to assess the overall water quality

Keywords: Water quality. pH, Temperature, Hardness, Electrical Conductivity

PP-95

ANALYSIS OF SILVER NANOPARTICLES PREPARED FROM HIBISCUS ROSA-SINENSIS LEAF EXTRACT THROUGH GREEN SYNTHESIS METHOD

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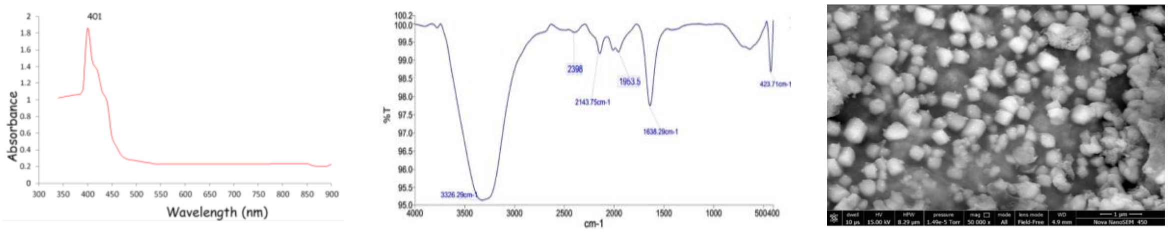
Abstract

The development of simple, nontoxic and eco-friendly method for the preparation of nanoparticles is an important step in the field of nanotechnology. Among the metallic nanoparticles, silver nanoparticles (AgNPs) gain much attention due to its chemical, physical and biological properties and applications. This study was carried out by synthesis and characterisation of silver nanoparticle using a composite leaf extract of Hibiscus Rosa-Sinensis. Various molecules (alkaloids, polysaccharides, alcoholic compounds, vitamins and amino acids) present in plant have ability to bio-reduction, formation and stabilization of silver nanopoarticles. The synthesis and characterization of silver nanoparticles was confirmed by UV-Visible spectrophotometer, Fourier Transform Infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM). UV-Visible absorption spectra of the reaction medium containing silver nanoparticles showed maximum absorbance at 401 nm. FTIR analysis confirmed reduction of Ag^+ ions to Ag^0 ions in synthesized silver nanoparticles. The SEM analysis showed the particle size between 1-50 nm and polydispersed spherical in structure. This study

revealed that the compounds from the extracts of *Hibiscus rosa-sinensis* L. are good reducing and stabilizing agents for the synthesis of silver nanoparticles.

KEYWORDS: Hibiscus rosa-sinensis, Silver nanoparticles, UV, FTIR, SEM, EDS.



(a) (b) (c)

Figure: a) UV-Vis Spectral analysis of AgNPs, b) FTIR spectrum of (HRSLE + Ag^+ ion), c) Scanning Electron Microscopic image of AgNPs.

Reference: (i) P.K. Tyag et.al., Materialstoday Proceeding, Vol.78, 1, 2023, 80.

(ii) P.Nie et.al, Ecotoxicology and Environmental Safety, Vol.253, 2023, 114636.

PP-96

BIO-REMEDIATION OF HEXAVALENT CHROMIUM USING PROSOPIS JULIFLORA BIOCHAR WITH CONCOMITANT DEGRADATION IS SOIL MICROBIAL FUEL CELL

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Abstract:

The stem of prosopis juliflora tree were chared by subjecting them to pyrolysis process at 450°C using muffle furnace. The obtained biochar was employed as a remediating material to adsorp Cr (VI) ions prepared from potassium dichromate solution of strength 0.2N. The extent of adsorption was determined by potentiometric titration method. The removal efficiency was calculated as 81% which provide viable solution for controlling primary

pollution. Then the products of adsorption study were carefully collected and admixed with soil in the ratio of 1:9 and the mixture was loaded in soil microbial fuel for subsequent Cr (VI) ion degradation with the benefit of electrical power generation. The soil microbial fuel cell (SMFC) was constructed in a glass beaker using meshed stainless-steel electrodes and the distilled water was employed as catholyte. The SMFC worked in the presence of toxic contaminant for 33 number of days with a study maximum potential 406 mV. The observation was noticed at the temperature of 25°C $^{\text{with}}$ the anodic and cathodic pH values of 7.4 and 7.7 respectively. Thus, the study concluded the power discharging ability of SMFC in presence of toxic contaminants. **Keywords:** Prosopis juliflora, Biochar, Cr (VI)ions, Remediation, Electrical Power and Soil microbial fuel cell.

PP-97

BIO-POWER GENERATION USING SOIL MICROBIAL FUEL CELL LOADED WITH HEXAVALENT CHROMIUM ION ADSORBED PROSOPIS JULIFLORA BIOCHAR

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Abstract:

The barks of the prosopis juliflora tree underwent charring through pyrolysis at 450°C using a muffle furnace. The resulting biochar was utilized as a remedial agent to adsorb Cr (VI) ions, which were derived from a potassium dichromate solution with a concentration of 0.1N. The degree of adsorption was determined via potentiometric titration resulting in a removal efficiency of 84%, offering a practical solution for mitigating primary pollution. Subsequently, the products of the adsorption study were carefully collected and mixed with soil at a ratio of

1:9. This mixture was then loaded into a soil microbial fuel for the subsequent degradation of Cr (VI) ions, with the added benefit of electrical potential generation. The soil microbial fuel cell (SMFC) was assembled in a glass beaker using meshed stainless-steel electrodes, with distilled water serving as the catholyte. The SMFC operated in the presence of toxic contaminants for 39 days, achieving a maximum potential of 424 mV at a temperature of 25°C. The observations recorded anodic and cathodic pH values of 7.3 and 7.8 respectively. Thus, the study concluded the SMFC's capability to discharge power in the presence of toxic contaminants.

Keywords: Biochar, Prosopis juliflora, Hexavalent Chromium Ion, Remediation, Electrical Potential and Soil Microbial Fuel Cell.

PP-98

CHARACTERIZATION, MICROBIOLOGICAL ACTIVITY AND DYE DEGRADATION OF ACTIVATED CHARCOAL SUPPORTED CADMIUM DOPED SnO_2 NANO COMPOSITES BY PRECIPITATION METHOD

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Abstract

In the present work, SnO_2, Cd/SnO_2 and $AC-Cd/SnO_2$ nanocomposites were prepared using precipitation method. The synthesized samples were characterized using X-ray powder diffraction (XRD), high resolution scanning electron micrographs (HR-SEM) with energy dispersive X-ray analysis (EDX), photoluminescence (PL) UV-Vis diffuse reflectance spectroscopy (DRS) and Fourier transform Raman analysis (FT-RAMAN). The XRD and SEM studies reveal that the synthesized SnO_2 nano materials have hexagonal wurzite structure with average crystalline size ~38 nm. Photocatalytic activity under ultra violet (UV) light exposure has been studied using methylene blue (MB) dye as test contaminant. A possible mechanism is proposed to explain the charge carrier recombination and interfacial charge transfer processes. It has been found the optimum amount of Cd^{2+} doping and increased adsorption ability of light due to high separation rate of photo induced charge carriers, which play an important role enhancing the overall photo catalytic performance significantly. Further its antibacterial activity against two gram positive and two gram negative bacterial strain and Antifungal also studied

Keywords: AC-Cd/SnO_2 Nanocomposite, Precipitation method, Characterization, Microbiological activity, Photo degradation.

PP-99

CONSTRUCTION OF HIGH-CAPACITANCE CARBONATE-RICH BIMETALLIC LAYERED (HYDR) OXIDES ONTO ZIF-67–Derived Co/CoO-N-CARBON HYBRID CUBES FOR HIGH-PERFORMANCE SYMMETRIC SUPERCAPACITORS

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Abstract

Herein, we fabricated carbonate-rich bimetallic layered hydr(oxides) (CoMnOx), which are primarily used as active materials for supercapacitors, using a simple hydrothermal method. CoMnOx was deposited onto cobalt oxide (CoO), which was produced by pyrolyzing ZIF-67 at 800 ◦C under N2 atmosphere. The Co/CoO cubes synthesized using carbonized ZIF-67 (ZIFC) were covered with CoMnOx shells with high reduction efficiency and abundant Co active sites and surface O species. The effects of the carbonate species present between the CoMnOx layers and at the surface of the hybrid CoMnOx@ZIFC materials were evaluated using PXRD and XPS. The peaks at the binding energies of 290 and 400 eV in the C 1s and N 1s XPS profiles of CoMnOx@ZIFC, respectively, indicate the presence of carbonate species and coordination of CoO and Co with the N-rich carbon materials, respectively. The FE-SEM images of CoMnOx@ZIFC revealed the partial decomposition of the cubic structure of ZIFC, which agreed with previously reported data. Moreover, the elemental composition of CoMnOx@ZIFC was confirmed using EDS mapping and point analysis. The CoMnOx@ZIFC electrodes exhibited a remarkable specific capacitance/capacitor of 963 F g− 1 /588 C g− 1 at 1 A g− 1 and excellent cycling stability over 1000 cycles, which was superior to those of previously reported MOF-derived carbonate-based materials in alkaline electrolytes. The CoMnOx@ZIFC||CoMnOx@ZIFC symmetric supercapacitor exhibited an energy density of 60.75 W h kg− 1 with a power density of 5947 W kg− 1 and an exceptional cycling stability (>99.5 %) after 3000 cycles.

PP-100

DFT OPTIMIZATION OF Au@ZnO CLUSTERS AND EFFECT OF CLUSTERS SIZE ON SURFACE-ENHANCED RAMAN SPECTROSCOPY (SERS) ACTIVITY

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Abstract

Distinctive electronic states in metal clusters exist at the interface of quantum and classical states. The characteristics and reactivities of molecules attached to metal clusters have a significant impact on those molecules. Gold nanoparticles are sighted for their countless physical, biological and pharmaceuticals applications. Zinc oxide is attracting significant attention from researchers due to its distinct characteristics and abundant uses in chemical sensors, transparent electronics and spin electronics. And also it has a great potential for numerous novel applications. Au@ZnO plays an important role in controlling shape and size. Geometrical optimization of clusters of ZnO and Au@ZnO are taken and optimized using Density Functional Theory (DFT). Optimized geomentries allow identifying the various properties and give insight into the interaction with the analyte molecules. The primary mechanism behind numerous improved spectroscopies like surface-enhanced Raman scattering (SERS), tip-enhanced Raman spectroscopy (TERS) and surface enhanced fluorescence (SEF) is a subject of major concern. SERS plasmonic phenomena is connected to the collective oscillation of the nanoparticle's conduction electrons. The ability to detect very few molecules, or even single molecules, has been made possible by the enormous amplification factors made possible by the SERS. The theoretical results in this aspect are to be discussed in detail.

Keywords: Density Functional Theory (DFT), surface-enhanced Raman scattering (SERS), Geometrical optimization, Metal clusters.

PP-101

GREEN SYNTHESIS OF MULTIFUNCTIONAL FLUORESCENT CARBON DOTS FROM GLORIOSA SUPERBA AND ITS APPLICATION AS Cr^{6+} SENSOR

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Abstract:

The attractiveness of using bio-pioneers to produce Fluorescent Carbon Dots (CDs) in an environmentally friendly manner for the use of heavy metal ion sensors is on-going research recent days. CDs were generated using green-pioneers (Gloriosa superba) in way of hydrothermal synthesis and then characterized the CDs using UV-Vis, Fluorescent spectral studies, FTIR, including this study reveal excellent water solubility, simplicity, and good biocompatibility. The synthesized CDs are subject to heavy metal ion sensor studies, the synthesized CDs exhibited an excitation-dependent emission manner, with an optimum emission wavelength at 407 nm excited at 272 nm. CDs were evaluated and shown to be effective FL sensors for detecting Cr6+ ions based on the FL quenching efficiency, demonstrating the special complex chelate between the metal ions and effective surface functional groups of CDs. Prepared C-Dots have been applied to detect Cr(VI) ions in aqueous solution. The proposed CDs extracted from *Gloriosa superba* flowers may have significant potential as a sensing probe for selective (Cr^{6+}) ions in the field of environmental water analysis.

PP-102

ENHANCED PHOTOCATALYTIC DEGRADATION OF DYES USING CuO/β-CD INCLUSION COMPLEX: SYNTHESIS, CHARACTERIZATION, AND FACTORS INFLUENCING PERFORMANCE

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Abstract

The host-guest inclusion complex is extraordinary photocatalysis against dye degradation process. In the present work, successfully synthesized Ethyl 4-(4-hydroxy-3-methoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate) (DHPM) via Biginelli reaction and it was characterised by ^{1}H-NMR, FT-IR, UV-Visible and fluorescence spectroscopy. Concurrently, CuO nanoparticles were synthesized through a wet chemical precipitation method and utilized for the modification of β-cyclodextrin. This modified form (CuO/β-CD) was characterised by XRD, SEM, EDX, TGA, UV-Visible and fluorescence spectroscopy. The CuO/β-CD used to prepare inclusion with DHPM. The stoichiometry and binding constant of the inclusion complex were determined using spectral data analysis. The free energy change (ΔG) was calculated. It is indicating a spontaneous and exergonic reaction. UV-Visible absorption spectra revealed a blue shift with increasing CuO/β-CD concentration. Moreover, CuO/β-CD prolonged the lifetimes of excited states of unreactive guests and facilitated electron transfer, thereby enhancing Rhodamine B degradation. The DHPM/CuO-β-CD complex exhibited significant photoactivity under visible light irradiation. The experiments were carried out to study the factors influencing the photocatalytic degradation such as the initial concentration of dye solution, catalyst concentration, illumination time and pH. The experimental results show that catalytic system bounded with CuO/β-CD exhibits superior photocatalytic activity than that of bare catalyst systems. The degradation rate was pH dependent.

Keyword: Nano particle, photocatalyst, Rhodamine B, dye degradation.

PP-103

ENHANCED METAL SENSING CAPABILITIES OF ETHYL 4-(4-HYDROXY-3,5-DIMETHOXYPHENYL)-6-METHYL-2-OXO-1,2,3,4-TETRAHYDROPYRIMIDINE-5-CARBOXYLATE (DHPM) INCLUSION COMPLEXES MODIFIED WITH SILVER NANOPARTICLES AND β-CYCLODEXTRIN

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Abstract

The synthesis of ethyl 4-(4-hydroxy-3,5-dimethoxyphenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (DHPM) through the multi-component Biginelli reaction is a straightforward process. The resulting DHPM compound characterized by ^{1}H-NMR, FT-IR, UV-visible, and Fluorescence spectroscopy techniques. Silver nanoparticles (Ag-NPs) were successfully synthesized and subsequently modified with β-cyclodextrin (β-CD) at room temperature. The modified form of β-CD (Ag/ β-CD) characterized by various analytical techniques, including FT-IR, UV-visible spectroscopy, Fluorescence spectroscopy, XRD, EDX, and TGA. The inclusion complex was prepared DHPM with β-CD and Ag/ β-CD. The stoichiometric ratio and binding constant (K) of these inclusion complexes were determined utilizing the Benesi-Hildebrand plot derived from absorption spectral data. Calculate the free energy change (ΔG) of inclusion complex, revealing the inclusion process to be exergonic and spontaneous. The resulting inclusion complex exhibited promising capabilities as a metal sensing probe, demonstrating selectivity and sensitivity towards Pb^{2+} sensing compared to other metals. Furthermore, a strong linear correlation between the complex and Pb^{2+} metal was observed, with an enhanced sensing mechanism noted during experimentation.

Keyword: DHPM, Nano particle, inclusion complex, Metal sensing.

PP-104

SYNTHESIS AND CHARACTERIZATION OF 4-(((4-NITROPHENYL) IMINO) METHYL) PHENOL AND INCORPORATED WITH PMMA/PEG/NiO DECORTATED β-CYCLODEXTRIN NANOFIBERS AND THEIR BIOLOGICAL APPLICATIONS

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Abstract

The electrospinning is a technique used to fabricate continuous nanoscale fibers with diameters in the sub-micrometer to nanometer range using a high-voltage power supply. PMMA/PEG nanofibers was produced in the ratio of 3:1 characterized regarding their morphology and chemical composition. Schiff base compound was synthesised from p-hydroxybenzaldehyde and p-nitroaniline. Strong intermolecular interactions are employed by supramolecular systems in the technique of electrospinning to form nanofibers. p-hydroxybenzaldehyde derivatives/cyclodextrin inclusion complex (P-OH derivatives/

CD-IC) were produced via electrospinning technique. Nickel oxide nanoparticles was prepared through co-precipitation method. P-OH derivatives/Nickel modified cyclodextrins inclusion complex was prepared through coprecipitation method their nanofibers mats fabricated. Structural, optical and magnetic properties of nanofibers were characterized by X-ray diffraction (XRD), UV-Vis absorption and Fourier transformed infrared (FTIR).Their morphological study of mats were investigated using SEM. Antibacterial studies of the nanofiber mats were tested against gram positive (*staphylococcus aureus*) and gram negative(*Escherichia coli*) bacteria. Ni Nps/ P-OH derivatives/Nickel modified cyclodextrin nanofibrous scaffold *in vitro* cytotoxicity using L929 cell were evaluated.

PP-105

SYNTHESIS AND CHARACTERIZATION OF MODIFIED SYRINGALDEHYDE DERIVATIVE FLUORECENT PROBE FOR METAL ION SENSING

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Abstract

In the present work, a cupric oxide decorated on β-cyclodextrin (CuO/β-CD) nanocomposite was synthesized by co-precipitation method. The CuO/β-CD nanocomposites were characterized by XRD, EDX, TGA, UV-Visible and fluorescence spectroscopy. Derivative of syrigaldehyde, (E)-2,6-dimethoxy4(((2methoxy phenyl)imino) methyl)phenol (DMIMP) was prepared and it is confirmed by ^{1}H-NMR, FT-IR, UV-Visible and fluorescence spectroscopy. Solid inclusion complex of DMIMP:

CuO/β-CD was prepared by co-precipitation and kneading method and it was characterized by using FTIR, ^{1}H NMR, XRD and SEM analysis. The stoichiometry and binding constant of inclusion complex was estimated using the Benesi-Hildebrand plot. A sensitive and highly selective, fluorescent “turn–on” fluorescence sensor for Zr^{2+} ions are reported by using a Syringaldehyde derivative: CuO/β- cyclodextrin (DMIMP: CuO/β-CD) solid inclusion complex in a methanol water system. In addition to the chemical studies, biological investigations were conducted to demonstrate the potential applications of the product.

Keywords: CuO/β-CD nanocomposites, DMIMP, “turn–on” fluorescence sensor.

PP-106

SYNTHESIS AND CHARACTERIZATION OF DAPSONE DERIVATIVE AND INCORPORATED WITH SnO_2/PVA AND β-CYCLODEXTRIN DECORTATED NANOFIBERS FOR BIOLOGICAL APPLICATIONS

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Abstract

The compound (1E,1'E)-N,N'-(sulfonylbis(4,1-phenylene))bis(1-furan-2-yl)methanimine) (SPFM), is primarily derived from dapsone and Furfural. These compounds have significant biological properties such as anti-inflamatory, anti- microbial, and antifungal activity. The synthesized compound undergoes characterization utilizing techniques such as ^{1}H-NMR, FT-IR, UV-Visible and fluorescence spectroscopy. In enhance the solubility of (SPFM), we synthesized tin oxide decorated on β-cyclodextrin (SnO_2/β-CD) nanocomposite

was synthesized by co-precipitation method. The SnO_2/β-CD nanocomposites were characterized by XRD, EDX, TGA, UV-Visible and fluorescence spectroscopy. SnO2/β-Cyclodextrin (SnO2/β-CD) is added to (SPFM) in an aqueous medium and formed the inclusion complexes (ICs). The stoichiometry and binding constant of inclusion complex was estimated using the Benesi-Hildebrand plot. Further, bio-composite materials in the form of nanofiber with (SPFM): SnO2/β-CD-ICs are obtained by using the electrospinning process with the help of polyvinyl alcohol (PVA). Nanofibers (NFs), in general, have various advantages like high surface-to-volume ratio, porosity, and mechanical and thermal stability. The surface morphology of (SPFM): SnO2/β-CD-ICs/PVA NFs, also revealed the uniform, bead-free NFs with 520.0–560.0 nm and exhibited the complete (SPFM): SnO2/β-CD-ICs dispersion in polymers at the nanoscale. The thermal stability and mechanical property of the material havealso been examined. The bacterial strains of Escherichia coli and Staphylococcus aureus showed antibacterial activity of the NFs using the disc-diffusing agar method. Overall findings indicate that these materials are useful in food packaging applications.

Keywords: Electrospinning, Nanofibers, SPFM: SnO_2/β-CD-ICs/PVA NFs.

PP-107

ENHANCING PHOTOCATALYTIC DEGRADATION OF PESTICIDES USING MODIFIED γ-CYCLODEXTRIN AND NANO-SIZED TiO_2-g-C_3N_4: SYNTHESIS, CHARACTERIZATION, AND COMPLEX FORMATION

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Abstract:

The pesticide usage holds greater significance for agricultural purposes, yet its impact on the environment, especially on soil and water, is profound and concerning. This research paper outlines the hydrothermal synthesis of nano-sized TiO_2 and g-C_3N_4, which were subsequently utilized to modify γ-cyclodextrin (γ-CD). The synthesised TiO_2 and g-C_3N_4 were determined by UV-visible spectroscopy, X-ray diffraction (XRD), Energy-dispersive X-ray spectroscopy (EDAX). To characterize the modified γ-cyclodextrin, various techniques were employed, such as UV, Fluorescence spectroscopy (FL), X-ray diffraction (XRD), Energy-dispersive X-ray spectroscopy (EDAX), Field-emission scanning electron microscopy (FE-SEM), and Fourier-transform infrared spectroscopy (FT-IR). The study also investigated the formation of inclusion complexes between a modified form of γ-cyclodextrin (TiO_2, g-C_3N_4, TiO_2-g-C_3N_4) and Methyl cinnamate (MC). The confirmation of these complexes was achieved using UV and FL spectroscopic techniques. Additionally, calculate the binding constant (K) and thermodynamic parameter (ΔG) for these complexes. Subsequently, the nanomaterials (TiO_2, g-C_3N_4), and their mixture (TiO_2-g-C_3N_4), along with the modified γ -cyclodextrin and their complexes, were employed in the process of photocatalytic dye degradation under visible light conditions (Natural- renewable source). The pesticides selected for degradation were Deltamethrin. The progress of the photo dye degradation reactions was monitored using UV-visible and fluorometric spectroscopy. Furthermore, the kinetics of the reactions were also determined in this study.

Keyword: g-C_3N_4, TiO_2, Methyl cinnamate, Inclusion complex, Pesticides, Degradation

PP-108

EXPERIMENTAL AND COMPUTATIONAL INVESTIGATION OF SYNTHESIZED TRANS METHYL CINNAMATE DERIVATIVES AND THEIR INCLUSION COMPLEXES

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Abstract

This study deals with the synthesis of Para hydroxy methyl cinnamate (PHMC) and Para ethoxy methyl cinnamate (PEMC) and it is Confirmed by ^{1}HNMR and FT-IR spectroscopy. The effect of solvent, different pH and β-Cyclodextrin on the absorption and fluorescence spectra of PHMC and PEMC have been investigated, the stokes shift of PHMC and PEMC are correlated with different solvent polarity scales to signify the hydrogen bond interactions are predominant. pH studies, PHMC's pKa and pKa* values of neutral and monoanion forms are detailed. Both the compounds inclusion with cyclodextrins and the complexes are characterized by experimentally (absorption, emission) and computationally (DFT) to determine the formation constant. The stoichiometric ratio determined by the Benesi-Hildebrand equation with their respective linear graph shows the 1:1 inclusion of complex formations. The solid complex was prepared and characterized by different analytical methods using FT-IR, ^{1}HNMR, XRD, DSC, and SEM.

Keywords: Methyl cinnamate, β-Cyclodextrin, fluorescence.

PP-109

Fe_2O_3-$C_{\beta CD}$/N-AQ NANOCOMPOSITE AS AN ANODE MATERIAL FOR SUPERCAPACITOR APPLICATIONS

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Abstract

The supercapacitor holds significant potential as the next generation of power sources for hybrid cars and portable devices. The characteristics of the electrode material have a major impact on the performance of supercapacitor, and much research has been done to find new electrode materials. In the present work, iron oxide doped inclusion complex derived activated carbon (Fe_2O_3-$C_{\beta CD/N\text{-}AQ}$) is prepared through hydrothermal method. The resulting composition, structural and surface morphology are evaluated by XRD, RAMAN and EDX analysis. The electrochemical performance of the prepared material studied by cyclic voltammetry and galvanostatic charge-discharge studies. Subsequently, the cyclic voltammetry study that the synthesized composite material delivers a higher specific capacitance of 320 Fg^{-1}. GCD analysis also reveals the good stability. The electrochemical impedance spectra revealed solution resistance (Rs) of 1.4Ω, 1.9Ω and 0.9Ω respectively. The result suggests that the Fe_2O_3-$C_{\beta CD/N\text{-}AQ}$ is a sufficient electrode material for supercapacitor application.

Keywords: Supercapacitor, Inclusion Complex, Iron Oxide

PP-110

Exploring Eco-Friendly and Green Synthetic Methods for 7-Hydroxy Flavone: Unveiling Laboratory Applications and Potential

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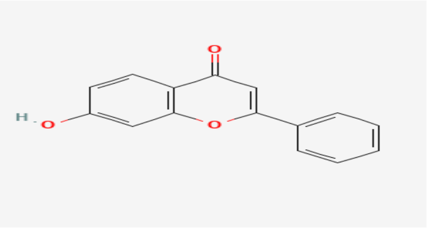

Abstract:

The synthesis of 7-Hydroxy flavone presents a promising avenue for exploration across multiple disciplines due to its diverse range of potential applications. This flavonoid derivative possesses notable pharmacological properties, making it a subject of interest in the pharmaceutical industry for its potential therapeutic benefits. Its antioxidant, anti inflammatory, and anticancer properties render it a candidate for drug development, particularly in the treatment of oxidative stress related disorders and cancer.

Furthermore, the synthesized 7-Hydroxy flavone demonstrates potential in the field of nutraceuticals and functional foods due to its antioxidant activity, which could contribute to health promotion and disease prevention. Its ability to modulate various cellular pathways suggests potential applications in dietary supplements targeting inflammatory and oxidative stress pathways.

In addition to its pharmacological and nutraceuticals applications, 7-Hydroxy flavone holds promise in materials science, particularly in the development of novel biomaterials and bioactive coatings. Its structural versatility allows for modifications that enhance its

compatibility with different matrices, making it suitable for applications ranging from drug delivery systems to tissue engineering scaffolds.

Moreover, the synthesized compound may find utility in agriculture as a natural pesticide or plant growth regulator, given its reported bioactivity against pests and potential to enhance plant resilience to environmental stressors.

Overall, the synthesized 7-Hydroxy flavone exhibits significant potential across various fields including pharmaceuticals, nutraceuticals, ma7&terials science, and agriculture, highlighting its versatility and the breadth of its potential applications. Further research and development are warranted to fully explore and harness its multifaceted benefits.

Keywords: 7-Hydroxy Flavone, Synthesis, Pharmacological Properties, Nutraceuticals, Materials Science, Agriculture, Antioxidant, Anti-inflammatory, Anticancer, Bioactivity.

PP-111

GREEN SYNTHESIS OF THIAMINE CATALYST FOR BENZOIN CONDENSATION

Laboratory Vs. Microwave Approach Methods

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Abstract:

Thiamine catalyzed Benzoin condensation reaction stands as a fundamental process in organic synthesis, facilitating the formation of valuable α-Hydroxy ketones. In the pursuit of sustainable methodologies, green chemistry principles have garnered significant attention, aiming to minimize environmental impact and enhance efficiency. This abstract outlines the synthesis of thiamine catalyst utilizing green chemistry methodologies, both through conventional laboratory approaches and microwave assisted synthesis.

The laboratory approach involves the utilization of eco-friendly solvents, optimized reaction conditions, and renewable starting materials. Thiamine, a naturally occurring vitamin, serves as an efficient catalyst, promoting the condensation of aromatic aldehydes into α-Hydroxy ketones. The synthesis route emphasizes the use of benign reagents, thus reducing waste generation and improving the overall sustainability of the process.

Additionally, microwave assisted synthesis offers a rapid and efficient alternative, further enhancing the green attributes of the process. Microwave irradiation enables precise control over reaction parameters, including temperature and reaction time, resulting in accelerated reaction rates and higher yields. This method underscores the principles of green chemistry by reducing energy consumption and enhancing reaction selectivity.

Comparative studies between the laboratory and microwave assisted approaches demonstrate their efficacy in synthesizing thiamine catalyst for benzoin condensation reaction. Both methods offer sustainable pathways for organic synthesis, aligning with the principles of green chemistry. Overall, the development of thiamine catalyst through green methodologies represents a significant advancement in promoting environmentally benign practices in organic synthesis.

***Keywords**:* Microwave heating, Green chemistry, Microwave synthesis, Microwaves.Thiamine catalyst, Benzoin Condensation, Green Synthesis.

AUTHOR INDEX