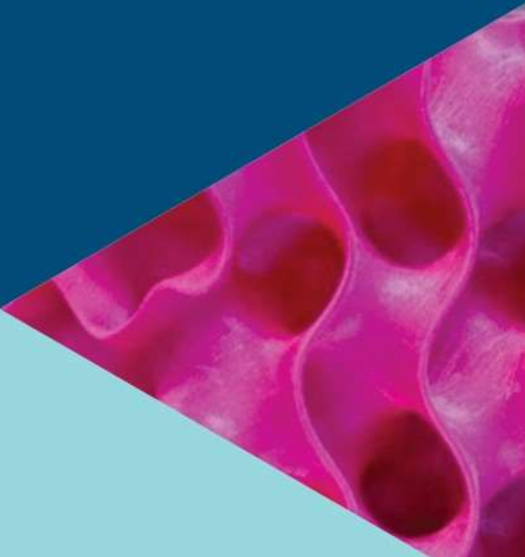
FRONTIER AREAS IN CHEMICAL TECHNOLOGIES

Volume-III

FACTs - 2022



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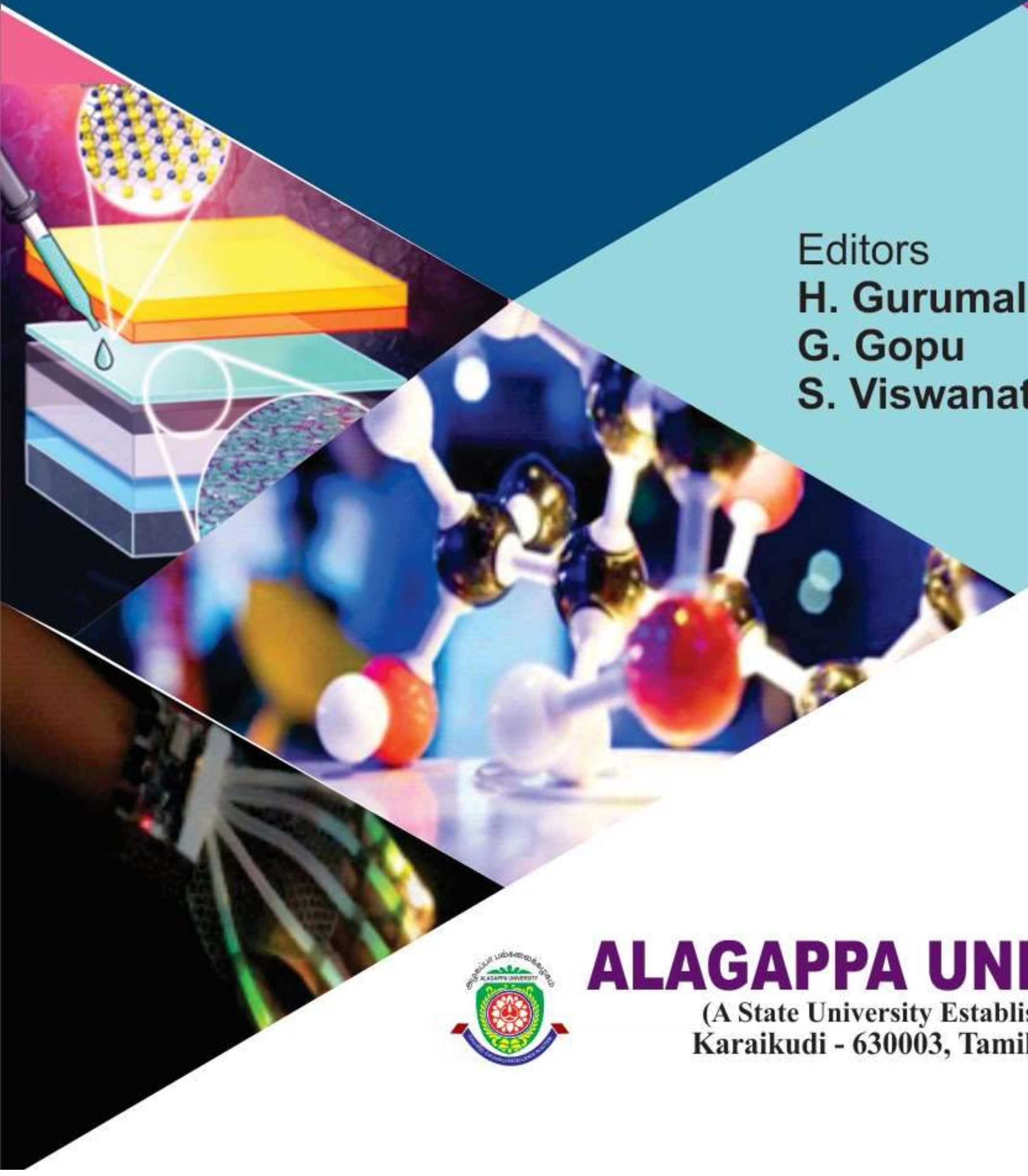

ALAGAPPA UNIVERSITY
(A State University Established in 1985)
Karaikudi - 630003, Tamil Nadu, India

Frontier Areas
in Chemical Technologies

Volume - III

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ALAGAPPA UNIVERSITY

[Accredited with A^+ Grade by NAAC (CGPA 3.36) in the Third Cycle]

KARAIKUDI – 630 003, TAMIL NADU, INDIA.

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Frontier Areas in Chemical Technologies

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Preface

Chemical technologies involving Green Chemistry, Material Chemistry, Electrochemistry, Textile Chemistry, Nanoscience, Computational Chemistry, etc., are the challenging as well as fascinating branches of advanced technologies and they find applications in almost all areas of Science and Technology. It is important for the researchers, educators and developers from academic institution and industries to know the research and recent developments that have been made on various aspects of Chemical and Electrochemical Sciences and Technologies. The present conference on **Frontier Areas in Chemical Technologies (FACTs-2022)** is the 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 and 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, Environmental chemistry, Supramolecular and Photochemical Technologies, Green Chemical Technologies and other allied technologies.

It is indeed a matter of great pleasure and satisfaction to the Editors to present this volume containing collection of extended abstracts of the presented in the International FACTS 2022 held at Alagappa University, Karaikudi during 16-18 February 2022. There are about 11 Invited Talks, 150 research abstracts for oral and 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 promoting the research culture among the young researchers. Our sincere thanks are to all the **Syndicate Members**, **Prof. S. Rajamohan,** Registrar and Authorities of Alagappa University, Karaikudi for their constant support and encouragement. The editors are pleased to acknowledge all the sponsors particularly RUSA 2.0. 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 extended abstracts in time.

We hope all the delegates had a pleasant stay in Karaikudi and stimulating discussions during the International Conference on FACTS 2022.

Editors

ALAGAPPA UNIVERSITY
Alagappapuram, Karaikudi - 630 003, Tamil Nadu, India.
(A State University Established by the Government of Tamil Nadu, Recognised by UGC)
[Accredited with A+ Grade by NAAC (CGPA: 3.64) in the Third Cycle]

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

FOREWORD

This compendium contains extended abstracts of the International Conference on Frontier Areas in Chemical Technologies-2022 (FACTs-2022). The conference is sponsored by the Alagappa University and RUSA 2.0 Scheme.

Chemical Industry is one of the oldest industries and playing an important role in the social, cultural, economic growth of a nation. Industries are providing basic needs of mankind (food, clothing, shelter) and become an indispensable part of our life. Chemicals in the form of Petrochemicals, Fertilizers, Paints, Soaps, Detergents, Perfumes, Pharmaceuticals and others are finding use in our daily life.

Extensive exploitation of chemicals in basic and applied fields has created threat to our environment. Sustainable development is an integral need of our eco-system. Thus, chemical technologies and their progress towards developing the Eco-friendly environment and rising the choice of existence of the humanity, solving environmental threats and conservation of natural resources are the order of the day. The evolution of appropriate chemical technologies should be in agreement with the needs and demands for the upcoming generation. In this focal task, this FACTs-2022 conference is organized by the Department of Industrial Chemistry during 16-18 February 2023.

The conference is designed with invited lectures from experts in India and abroad, oral and poster presentations by the participants. This conference can assemble researchers and experts working in this field to share their best knowledge in the development of Science & Technology. This conference can provide a platform for participants to share and handle recent findings of their research linking topics related to chemical technologies and enlighten new ideas. The invited lectures and research papers presented at FACTs-2022 would serve as an important collection of research ideas/inputs in the field of Chemical Technologies. The research deliberations / information can be a resource information for researches, academicians and industrialists.

Organization of conference requires the dedicated efforts of many people. I congratulate Dr. H. Gurumallesh Prabu, Professor & Head, Department of Industrial Chemistry, for taking the efforts to organize this International Conference. I appreciate the convener, organizing secretary and members of the conference committee for their diligent and professional work. I thank all invited speakers for their research contribution. I wish all the speakers and delegates to have bountiful interaction and memorable activity at Alagappa University.

14/02/2023
Prof. G. Ravi

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1. Invited Talks

1.1 Overview of strategies of development and applications of voltammetric biosensors

S. Morais

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Electrochemical biosensors integrate the sensitivity of electrochemical transducers with the high selectivity of biological recognition. The biological element recognizes its analyte causing a biocatalytic or binding reaction, which yields an electrochemical signal (registered by a transducer), that is related with the analyte concentration. Biocatalytic devices incorporate enzymes, whole cells, or tissue slices that identify the target analyte and originate electroactive species. Affinity devices are based on a selective binding interaction among the analyte and the biological component such as an antibody, nucleic acid, or a receptor. The past and recent accomplishments of nanotechnology assure that good (immobilization) stability, ultrahigh sensitivity, good selectivity, low detection limit, fast response time, and miniaturization of the biosensing platform can be reached. Biosensors correspond to an intense growing field of research, which is reflected by the large number of studies that have been published in the recent years and by the rising number of these low cost technological tools that are, nowadays, applied in diverse sectors, such as food quality and safety, environmental pollution control, industrial process monitoring and control, biotechnology, pharmaceutical and clinical analysis, among others [1-9]. Additionally, the development of biosensors contributes to answer to technological, socioeconomic, and environmental challenges that are clearly outlined in the 2030 Agenda for Sustainable Development. Several case studies will be discussed.

Acknowledgements

Simone Morais is grateful for the financial support by the project NATURIST 2022.07089.PTDC funded by the National Funds through Portuguese FCT - Foundation for Science and Technology. The support through UIDB/50006/2020, UIDP/50006/2020 and LA/P/0008/2020, from the Fundação para a Ciência e a Tecnologia (FCT)/Ministério da Ciência, Tecnologia e Ensino Superior (MCTES) is also acknowledged.

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1.2 Electrochemical immunosensing of food allergens

M. Freitas[1], M. del Rio[1], A. Carvalho[1], C. Oliveira[1], D. Guimarães[1], R. Torre[1], P. Rocha[1], E. Costa-Rama[2], M. Neves[3], H. Nouws[1], C. Delerue-Matos[1]*

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Food allergy represents a public health problem since it affects millions of people worldwide. There is currently no treatment for this problem; it’s recommended to eliminate foods or food ingredients from the diet that could result in allergic reactions. Therefore, the EU established a priority list of ingredients or products that can cause allergies and obliges the indication of their presence on food labels. This plays an important role in protecting manufacturers and consumers. However, indications such as "may contain allergens" are frequent and unnecessarily restrict the diet of allergic consumers, reduce the credibility of the label, and result in a loss of quality of life.The established methods for the analysis of allergens are often time consuming, expensive, and require sophisticated equipment, which prevents effective screening and may compromise their acceptance in companies with limited resources. This project intended to respond to these challenges by developing small, cheap, and easy to handle electrochemical immunosensors that can selectively detect trace amounts of allergens in food products and ingredients. The developed sensors were fully validated and can be used for the analysis of several major allergens of peanut, shrimp, fish, egg, and celery. These sensors can be very useful for the food industry because they allow key decisions to be taken throughout the entire production chain.

1.3 Preparation of recycled ultrafine graphite scrap by ball milling and bead milling from industrial graphite waste

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An industrial graphite waste obtained from fabrication process of graphite block was undergo particle size reduction process by using ball milling and bead milling. Dispersing agent was found to play an important role on the particle size reduction process in both techniques. A system of single surfactant and mixed surfactant of sodium dodecyl sulfate (SDS), lignosulfonate (LS) and mixed SDS+LS were investigated. The quality of milled particle was judged from grinding performance, particle size distribution and grinding time. Oven dried ultrafine graphite was mixed with amorphous carbon and coal tar pitch prior to die compaction and carbonization, yielding carbon block. Density, hardness, flexural strength and electrical conductivity were measured against carbon block.

1.4 Microplastics and related chemicals in the environment: global concern and multiple challenges

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Plastic has long been a fundamental material in modern society, and every year more than 300 million tonnes are produced. Plastic is a single word for a complex reality, comprising a wide variety of polymers and additives with different chemical and physical properties. Plastic pollution in various forms has emerged as the most serious environmental threat. Microplastics have become ubiquitous and detected in marine and fresh water, soils, air, food, and several species including humans (1). Nowadays, it is evident that microplastics release toxic plastic additives and can adsorb various chemicals, thus serving as sinks for various hazardous compounds, increasing their bioavailability, toxicity, and transport in the environment. In addition, there is an emerging threat of trophic transfer of microplastics to humans and other higher animals (1,2). The polarity of the microplastic surface allows interactions (sorption and desorption) with surrounding chemicals that can be facilitated in environments where plastics are degraded by UV radiation and temperatures (3). To address these concerns, it is essential to have consistent data on the assessment of microplastics and related chemicals. The work to be presented will focus on i) analytical methods for the extraction and analysis of MP in environmental samples; ii) Microplastics and pesticide interactions in an aquatic environment and iii) ecotoxicological effects of MP and related chemicals in a terrestrial environment.

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1.5 Electrochemical sensors and biosensors through Polish -Indian cooperation

Hanna Radecka[*]

[*] Professor Emeritus, Biosensors Department, Institute of Animal Reproduction and Food Research, Polish Academy of Sciences, Tuwima 10, 10-748 Olsztyn, Poland; E-mail: h..radecka@pan.olsztyn.pl

Biosensors Department leading by Professor Jerzy Radecki has been concentrated on the development of electrochemical sensors and biosensors. Due to his extremely scientific involvement and the ability to establishing cooperation, the numerous, novel immunosensors genosensors and anion sensors have been developed with very important participation of young scientists from India. The most successful examples of biosensors based on ion – channel mimetic mode and based on redox active layers will be presented. Their working principles, analytical parameters and ability for application for the direct electrochemical detection of viruses as well as antibodies in the natural physiological samples will be discussed. The recognition of anions in water medium is still a challenging task. The synthetically produced receptors has been successfully applied for determination of Cl^- and SO_4^{-2} in highly diluted water medium (in the picomolar range). The results obtained allowed establishing the mechanism of communication between the redox center and receptor anion complex as well as analytical signal generation.

Keywords: immunosensors, genosensors, anion sensors, redox active monolayers, ion-channel mimetic mode

1.6 Point of Care Diagnostic Devices - Opportunities and Challenges

Dr. *Muthukumar Chockalingam*

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Point-of-care (PoC) diagnostic devices enable rapid detection of specific analytes present in the clinical samples and help physicians in the process of early diagnosis and interventions. Although great achievements have been made in the field of PoC research, there are still some major challenges in translation of the research into viable products. In this report, a SWOT analysis on the progress of PoC device development has been carried out. A wide range of PoC concepts including invasive and particularly non-invasive methods have been considered for the detection of important biomarkers/early symptoms of acute health problems or causes of acute health problems. In the invasive method, the existing laborious testing methods are explored for conversion into compact point of care devices for rapid detection of the analytes in the samples. In the non invasive method, a latest tool of computational algorithms powered by data sets and artificial intelligence has also been explored to predict acute health problems such as developmental disorders, cognition health, cancer and various other acute health problems at a very early stage to begin timely interventions. The report also discusses the challenges in translation of the PoC research and strategies for bringing out the PoC products to the market.

1.7 Nanostructured materials for Energy harvesting from waste heat

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Thermoelectrics (TE) is a reliable technology to convert the waste heat into electricity. Nanostructured TE materials have attracted the researchers due to their high performance compared to their bulk counterpart caused by increased phonon scattering and quantum confinement effect. The oxide TE materials show the promising improvement in recent years. Moreover, the oxide materials are non-toxic, environmental friendly and ease to process as a device. Thermoelectric properties of selenide and telluride based semiconductor nanomaterials have been investigated [1]. Moreover, a novel series of BixCo3-xO4 (0 ≤ x ≤ 0.2) and BixZnCo2-xO4 (0 ≤ x ≤ 0.2) nanocrystals have been investigated as a function of Bi content. The structural, morphological and compositional properties of the prepared materials are studied by XRD SEM and EDS analysis. The variations of electrical resistivity and Seebeck coefficient of BixCo3-xO4 (0 ≤ x ≤ 0.2) and BixZnCo2-xO4 (0 ≤ x ≤ 0.2) at different temperatures were studied. It was observed that the electrical resistivity decreased till x ≤ 0.05 due to the substitution of Bi ions in Cobalt lattice and increases at higher x values (0.05 ≤ x ≤ 0.2) for BixCo3-xO4 due to the formation of secondary phase of Bi2O3. The Bi substitution has considerably reduced the electrical resistivity by one order when completely dissolved in the cobalt oxide lattice at lower x values. The electrical resistivity of BixZnCo2-xO4 decreased with x value and slightly increased for the sample with x value ≤ 0.1. Bi0.2Co2.8O4 sample exhibits the power factor of 0.025 μWm−1K−2 at 530 K, whereas Bi0.1ZnCo1.9O4 shows the high-power factor of 2.3 μW K−2 m−1 [2] nearly at the same temperature. The experimental results revealed that Bi substitution in BixCo3-xO4 and BixZnCo2-xO4 is a promising approach for improving their thermoelectric properties.

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1.8 Flexible Electrochromic display devices: Role of conducting polymers for the fabrication of flexible electrodes

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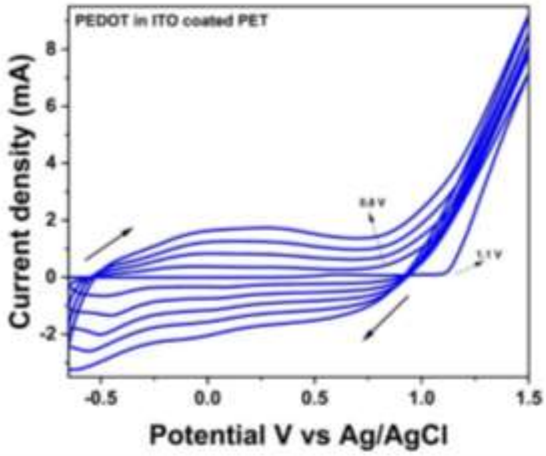
Conducting polymers are a class of organic electrochromic materials which gain importance rapidly, due to the combination of processability and low cast, fast response times, and optical contrasts and the ability to modify their structure to create multicolor electrochromic behavior, which will be more beneficial for the development of flexible devices. Direct electrochemical deposition of thin film of conjugated conducting polymer film is adopted to fabricate the flexible electrodes of definite dimension instead of inorganic electrochromic materials. In the present talk will cover the preparation and fabrication of electrochromic layers on ITO coated transparent flexible PET substrate [area= 1x1 & 2x cm2] by chemical and electrochemical route. The flexible films are examined with spectro-electrochemical study, electrochromic switching (both normal & flexible mode) kinetics and structural morphology characterizations for the suitability of the device fabrication. Vacuum filling process of gel electrolyte is adopted to achieve the bubble free electrolyte during the device fabrication, which results high optical contrast ratio, fast switching, long cycle life and low energy consumption.



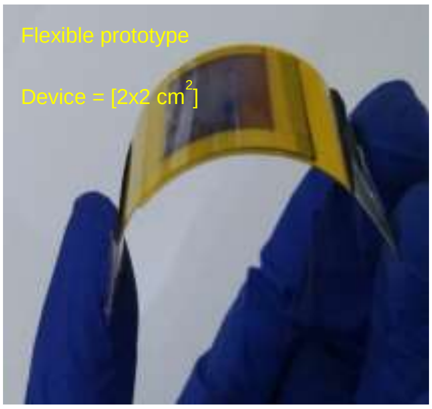


Fig.1: Electrodeposition of PEDOT film on flexible PET; Image- flexible electrochromic device

Key words: Conducting polymer, electrodeposition, Flexible electrode, Optical study and Electrochromic device.

1.9 Structural defects of 2D MoS_2 nanosheets and their arsenic adsorption behaviors from water

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Generally, structural defects provide extraordinary opportunities to tailor the intrinsic properties and create new functionalities. For 2D materials, structural defects have been found to have strong influence on the electron−electron interactions. Different types of defects in MoS2 nanosheets were found playing important roles in various applications. Arsenic contamination in natural water is a worldwide problem. Arsenic mostly exists in two different oxidation states, i.e., arsenate (AsO43-) and arsenite (AsO33-), in natural water, in which arsenite is fifty times more toxic than arsenate. Molybdenum disulfide (MoS2), a 2D material, has shown a wide range of mechanical, physicochemical, electrical, and adsorption applications, owning to its active sulfur functional groups. To accelerate the adsorption densities towards anionic pollutants, the highly stable MoS2 is modified as defective by the incorporation of oxygen atoms. In this study, we aimed to synthesize a metal (La) loaded O-rich MoS2 nanosheets through an in-situ hydrothermal reaction for the adsorption of toxic arsenite and arsenate ions from water and compared their efficiency with commercially obtained La(OH)3/MoS2 materials. The intercalation/surface loading of La at different equivalent ratios into a few layered O-rich MoS2 nanosheets were successfully synthesized and characterized through several spectro-analytical techniques. From the FE-SEM and TEM images that obvious ripples and corrugations can be observed, revealing the ultrathin nature of the nanosheets, and the La-particles were decorated over it. The La-ions tend to bind with the O-moiety in the MoOxS2-x, rather than S by well understood HSAB principle and the S atoms are free for the capture of arsenite ions. Loading La-ions in the defective structure intended to adsorb arsenate ions from water through multiple mechanisms. Reusability of the material after seven cycles is yet another merit of the developed material towards arsenic removal. The results indicated that La-incorporated O-rich MoS2-x has considerable potential candidates for the decontamination of arsenic from waters.

Keywords: 2D material; Oxygen incorporation; Metal insertion; Arsenite-arsenate; Adsorption.

1.10 Novel Co-reactants for Electrochemiluminescence Sensing Application

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Electrochemiluminescence (ECL) also called as Electrogenerated chemiluminescence, is a highly sensitive process in which electrochemically generated reactive intermediates combines to undergo high-energetic electron-transfer reactions to form excited states, which emit light without applying any external source of light. Generally, Generation of ECL emission follows primarily via two reaction mechanisms such as (1) annihilation and (2) co-reactants. Each of these mechanisms offers different advantages and relies on different pathways to generate the excited state at electrode interface that ultimately emits light. In annihilation mechanism, the reduced and oxidized species are both generated in the vicinity of the electrode surface by wide range potential sweep. The co-reactant ECL is usually generated by the reaction between the luminophore species and an additionally added assistant reagent (co-reactant) by one directional potential scanning (either anode or cathode direction). The use of co-reactant can produce more intense ECL emission than annihilation reaction. ECL with co-reactant produces highly intense signals in both aqueous and non-aqueous solutions because it needs a narrow potential window to generate stable reactive intermediates for annihilation between oxidized and reduced species. All commercially available ECL analytical instruments are based on this pathway. According to the generated intermediates and the polarity of the applied potential, the corresponding ‘‘co-reactant ECL’’ can be classified as ‘‘oxidative-reduction’’ and ‘‘reductive-oxidation’’ –ECL. The energy required to generate an excited molecule can be calculated using enthalpy factor (ΔH). The required energy to obtain an excited state molecule should be equal or greater than 2.1 eV.

$$\Delta H = \Delta G + T\Delta S = (\boldsymbol{E}^{0}_{\boldsymbol{R}/\boldsymbol{R}^{\cdot+}} - \boldsymbol{E}^{0}_{\boldsymbol{R}/\boldsymbol{R}^{\cdot-}}) - 0.1\ \mathrm{eV}$$

Using this kind of unique ECL technique offers a grand avenue to understanding the fundamental properties like physicochemical and electrical properties of organic molecules, semiconducting nanostructured materials, quantum dots, metal clusters and etc. Also, this ECL emission could be used in the estimation of biologically important molecules especially at the single molecular level by either selective quenching or enhancing ECL signal.

1.11 Sustainable Water Electrolyser Technology: A key to India’s Energy Transition Dream.

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Realising the hydrogen economy is a prime strategy towards decarbonisation to mitigate the climate change problem. India aspires to be a responsible state joining hands with the world towards this global effort. India's recent announcement of the National Hydrogen Energy Mission(NHEM) is a major boost towards the ineludible energy transition. A missing block in the green hydrogen 'jigsaw' is a sustainable technology to generate it. The talk will cover various aspects of the hydrogen economy, water electrolysers, and CSIR's mission to develop indigenised technologies for sustainable hydrogen generation at a highly competitive cost.

2. Biosensors and Chemical sensors

2.1 Design and development of electrodeposited Pd-thin film electrodes for acetaminophen detection

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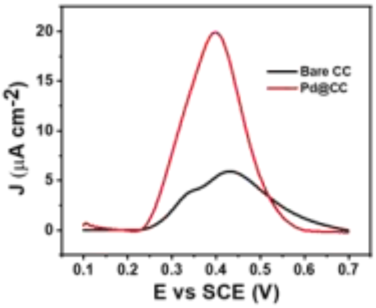
The present work is mainly focused on the preparation of eco-friendly electrodeposited flexible electrode using ammonia complex without any surfactant additives. Herein, Pd electrodeposition was carried out on carbon cloth (CC) and applied for electrochemical sensing applications. Further, cathode current efficiency and rate of film growth were calculated using Faraday's law of electrolysis which helps to improve the quality of deposited Pd. The surface morphology, crystalline structure, topography, elemental composition and oxidation state of elements were analysed by FESEM, XRD, AFM and XPS characterisation techniques. The electrochemical sensing performance towards acetaminophen (ACAP) in neutral medium (pH 7.0) were evaluated using cyclic voltammetry (CV) and differential pulse voltammetry (DPV). PdCC modified electrode shows an enhanced electrocatalytic activity for the oxidation of ACAP with lower oxidation potential with a wider linear range of 5 – 6000 µM along with an LOD of 0.942 µM. The PdCC modified electrode has achieved good stability, reproducibility, reusability and anti-interference ability towards the sensing of ACAP.



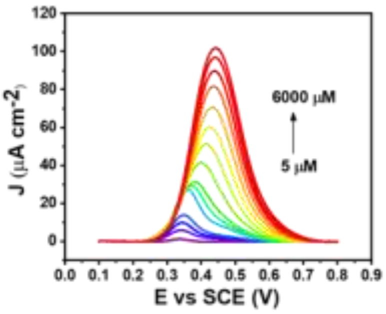


Figure: DPV response of bare CC and PdCC with the existence of 1 mM ACAP and (B) DPV concertation effect.

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2.2 Acridinedione-based fluorescent probe for the detection of Cr^{6+} Ion

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The acridinedione (AR1) was synthesized in excellent yields and environmentally friendly conditions by a one-pot multi-component reaction using 1,3- dicarbonyl compound with aromatic aldehydes and substituted amines in the presence of ethanol used as a solvent. The synthesized compounds were characterized by FT-IR, NMR, HRMS, and SC-XRD spectral techniques. The receptor AR1 shows the colorimetric response from yellow to colourless and fluorescence “turn-off” with Cr6+ ions under UV light. Both the UV-Vis and fluorescence studies confirmed the formation of a 1:2 stoichiometry complex. The sensor activity was found to be high in the basic pH (6.0- 11.0) without any interference from other interfering ions. Therefore, AR1 can be used as a promising probe for the detection of Cr^{6+} content in the semi-aqueous phase.

Keywords: Acridinedione, Chromium IV ion, Fluorometric detection, and Chemosensor.

2.3 Fabrication and Characterization of Nanostructured Porous Silicon with Immobilization of Biomolecules for Sensor Applications

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The High Sensitive and Selective Nanostructured of Porous Silicon (PS) layers prepared from p-type silicon wafers of (100) orientation by electrochemical etching method and well established fabrication process. SEM and PL studies were carried out to characterize the surface morphological and efficient visible optical properties of porous silicon. The chemical mechanism of coupling reaction on porous medium – liquid interaction for Si-(C=O) of amide – I stretch bond and Si-(C=N) of amide –II stretch bond characterized the deposition of biomolecules on the etched and oxidized porous treated silicon surface by Fourier transform infrared spectroscopy studies. The important role of molecule on etched porous silicon and oxidized porous treated silicon were characterized that the isolated pore walls are fascinated by the infiltration of biomolecule into the pores treated porous silicon layer. The new coverage of surface passivation of porous silicon was functionalized almost prominent intensity peak value that the porous silicon layer gave some strong and weak evidences of the quantum confinement effect in Si-H groups of the optimized Immobilization of biomolecules. The porosity of porous silicon was estimated by geometrical method using the size and shape of pore in the binary parameters obtained from SEM images. In order to concurrent between the refractive index gives dielectric of porous silicon, porosity and immobilization of biomolecules fraction calculated in the four components Bruggeman effective medium model (void, silicon pores, oxide and biomolecules). The spontaneous imbibition weight for the porous medium imbibed for the Cysteine, Leucine and Valine as wetting liquid onto etched and oxidized porous silicon surface by photoluminescence studies. The changes light emission over the treatment of nanostructured porous silicon provoke for absorption of the hydrogen atoms and localised states related to Si-O bonds desorption. and results suggest that could be realized in optical nanomaterial as well as biosensor applications.

Keywords: nanostructured porous silicon, nanomaterials, biomolecule, biosensor applications

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2.4 Surface engineering of Hollow Carbon Tubes via Heteroatom Doping Approach for Electrochemical Detection of Diphenyl Amine

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To design and develop a facile synthesis of hollow tubular carbon-based materials with higher catalytic performances are remains challenging. Herein, self-sacrificing template strategy is employed for the construction of graphitic layer wrapped hollow carbon nanotubes (CNT) encapsulated with nitrogen and sulphur heteroatoms. Surface engineering of nitrogen and sulphur codoped mesoporous hollow carbon nanotubes (NSCNT) is described, and synergistic effect of heteroatom doping and porosity tuning upon the electrochemical performance is demonstrated for the effective detection of diphenyl amine (DPA). Differential pulse voltammetry was employed as an electrochemical tool to assay DPA using NSCNT-0.5/GCE with an increased sensitivity of 3-fold compared with bare. Benefitting from abundant catalytic active sites and faster electron transfer kinetics, the NSCNT modified electrode covered a wide range of concentration 5-500 μM and achieved a lower LOD with appreciable sensitivity. Moreover, the impact of negligible effect over potential interferents, reproducibility measurements and operational stability had augmented much effect on DPA sensing which clearly makes it as ideal sensing device feasible for technical analysis. Real sample analysis was scrutinizing the excellent efficiency and reliability of proposed sensor with fruit samples for the detection of DPA with peerless recovery range.

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2.5 Theoretical Analysis of the Steady- State Behaviour of Urea Biosensor for Non-linear Equations

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A mathematical model for the dynamic behaviour of urea biosensors under steady-state settings at non-stationary enzyme kinetics is reported. It is based on Michaelis-Menten kinetics and nonlinear reaction-diffusion equations. The Akbari-Ganji method (AGM) derived a simple and concise analytical expression for substrate, inhibitor, and product. This powerful algebraic technique assumes an initial solution with unknown coefficients that satisfy both the initial conditions and the differential equations. Furthermore, the analytical results of all parameter values are compared with numerical simulation. The analytical and numerical solutions have a satisfactory agreement.

2.6 Theoretical Analysis of Mathematical Modelling on Potentiometric Biosensors using Akbari Ganji Method

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A mathematical model of potentiometric enzyme electrode biosensors under steady-state conditions is discussed in this article. This model is based on Michaelis-Menten kinetics, which describes the substrate and product concentrations within the enzymatic layer. The two coupled nonlinear steady-state reaction-diffusion equations are solved using the Akbari Ganji Method. This paper reports the approximate analytical expression for the substrate, product and flux concentration. The analytical solutions are compared with numerical simulation for the experimental values of parameters using the Scilab/Matlab software. Good agreement between the analytical and numerical solutions is noted.

2.7 Theoretical analysis of steady-state concentration in transport processes of amperometric biosensor using Akbari-Ganji method

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The theoretical model of the carrier-mediated transport processes is discussed in this paper. This model is based on the reaction-diffusion equation containing non-linear terms related to the reaction rate. An approximate analytical expression for the steady-state concentrations of substrate and product is discussed. The Akbari-Ganji method is employed to solve non-linear reaction-diffusion equations. The analytical results are compared with numerical simulations using MATLAB.

2.8 Mathematical Modeling of PPO-modified microcylinder biosensor for Planar electrode: Akbari Ganji Method

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An electroenzymatic method using a modified microcylinder electrode in which polyphenol oxidase occurs for all values of catechol and o-quinone concentrations is theoretically described. The Michaelis-Menten kinetics of the enzymatic reaction is modelled using a system of reaction-diffusion equations with a nonlinear factor. The system of nonlinear differential equations representing diffusion coupled with Michaelis-Menten kinetics is solved using the Akbari Ganji Method in this study. The approximate analytical expression for the dimensionless concentration of catechol and o-quinone and dimensionless current in kinetic parameters. Additionally, the relationship between the concentration of catechol and o-quinone is also obtained.

2.9 Tungsten Oxide and Gold Nanoparticle Interface for Label free Electrochemical E-Coli DNA Sensor

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Tungsten oxide-Gold nanoparticles (WO3-Au) composite was synthesized by hydrothermal method and modified the gold electrode by a simple drop-casting method. The electrochemical label-free Escherichia Coli (E-Coli) DNA sensing is made in presence of 1 mM potassium ferri/ferrocyanide K3[FeIII(CN)6]3-/K4[FeII(CN)6]3- by cyclic voltammetry and electrochemical impedance spectroscopy techniques. The WO3-Au composite is characterized by UV- visible, Fourier-transform Infra-red (FT-IR), X-ray diffraction, X-ray photoluminance spectroscopy, and transmission electron microscopy (TEM) techniques. WO3-Au showed higher discrimination efficiency for un-hybridized (single-stranded DNA) and hybridized (complementary hybridized, dsDNA) than the similar literature, indicated by the wide linearity 10-18 to 10-6 M observed for complementary dsDNA sensing. The specificity of the sensor is demonstrated by the observation of low impedance signals for non-complementary and single and double base mismatched dsDNA compared to the complementary dsDNA.

Keywords: tungsten oxide, gold nanoparticle, label-free, E-coli, DNA, electrochemical

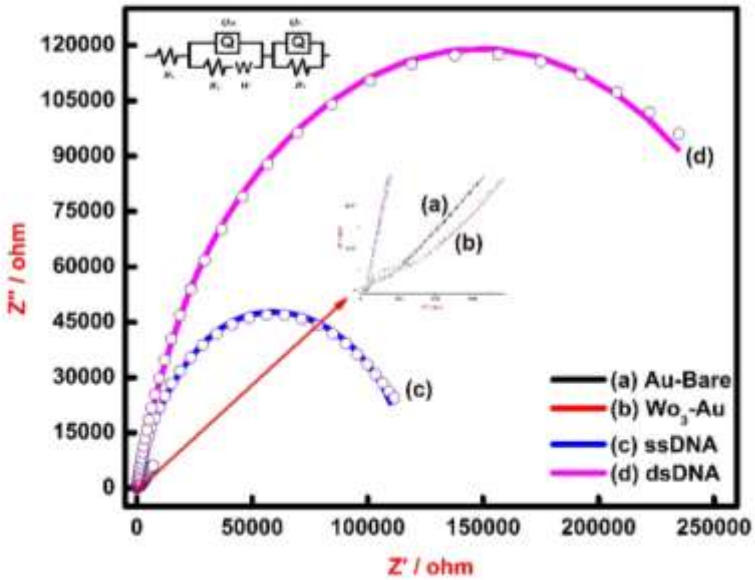

Figure 1- Electrochemical impedance behaviour of Modified gold electrode measured in PBS buffer (pH 7.4) in presence of 1mM K_3/ K_4 Fe[(CN)$_6$]$^{3-/4-}$ in the frequency range of 100KHz to 1KHz and applied potential 0.16v.

2.10 Cholesterol based binary lipid gold nanoparticle composite for ultrasensitive Label free E-Coli DNA sensing

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Lipid layer containing cholesterol gold nanoparticle and cationic, neutral and anionic lipid was prepared on gold electrode using mixed monolayer cushion for ultra sensitive electrochemical label free DNA and unprocessed whole E.coli bacterial cell detection in presence of K3[Fe(CN)6]/K4[Fe(CN)6] in physiological buffer. Cholesterol and gold nanoparticles interactions were characterized by dynamic light scattering (DLS) technique, cyclic voltammetry (CV), electrochemical impedance (EIS), and Fourier infrared transform (FT-IR) and Transmission electron microscope (TEM) techniques. Insulation property of mixed monolayer towards K3[Fe(CN)6]/K4[Fe(CN)6] is influenced by *the* presence of lipid-gold nanoparticles. DNA hybridization studies indicate higher discrimination efficiency (75±3%) between the un-hybridized ssDNA and hybridized dsDNA for the binary cationic/cationic lipid-gold composite compared to the discrimination efficiencies 20±3% and 5% noticed for other composite membranes cationic/anionic, cationic/neutral and anionic/neutral membranes constructed on thiol monolayer cushion. The sensor showed a wide linear range from 10-9 to 10-19 M with lowest detection limit (LOD) of 10-19 M and limit of quantification (LOQ) 10-17 M. E.coli DNA was used as a model system. For real sample validation, Staphylococcus, Enterococcus and E.coli were isolated and used for the direct and selective sensing of whole E.coli cell at 106 CFU/mL by label free impedance technique. (For the studies on cross reactivity of the sensors for other pathogens like Staphylococcus and Enterococcus reveal specificity of the bioelectrode for E.coli cell at 106 CFU/mL by label free impedance technique.)

Keywords: Cholesterol, AuNP, DNA, label free, electrochemical, cationic lipid

2.11 Electrochemical immunosensor for HIV biomarker in blood serum.

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An electrochemical immunosensor for detecting HIV p24 in blood serum samples was developed. Gold nanoelectrode ensembles (GNE) were prepared by electroless deposition of the gold within the 50 nm pores of polycarbonate particle track-etched membranes. A simple controlled solvent etching procedure based on the solubility of polycarbonate membranes in solvent mixtures is adopted for the fabrication of the nano electrodes(Fig. 1). GNE was used to attain good conductive support for the immobilisation of anti-HIV -p24 antibody molecules. The percentage peak current reduction showed a linear increase vs. log of p24 concentrations in the range between 2 and 900 pg·mL-1 (Fig. 2). The calibration curve presented wide linearity, good sensitivity (slope = 20.6 % IpR /mL·ng-1) and good distribution of the data with a correlation coefficient (r) of 0.9. The limit of detection (LOD) was calculated as the lowest concentration of HIV-1 p24 that gives an analytical signal three times higher than the standard deviation of the analytical signal obtained in the absence of HIV-1 p24 under identical conditions. The LOD value thus obtained was 1 pg·mL-1. Additionally, the reusability of the immunosensor was assessed. The immunosensor, once used for 10 pg·mL-1 HIV-1 p24 detection was immersed in 0.1 M glycine-HCl solution pH 3 for 20 minutes with the aim of breaking the antibody-antigen linkage. Then it was used for HIV-1 p24 detection again. After ten regeneration cycles, the current response of the immunosensor decreased by 20 %, demonstrating a successful regeneration of the immunosensor. So, the analytical characteristics combined with the simplicity of the proposed immunosensor make an interesting tool for HIV-1 p24 determination. Even more, considering label-free detection which avoids the need for expensive enzyme-linked antibody for recognition or functionalised nanomaterials for signal amplification, can reduce the operational complexity and assay cost.

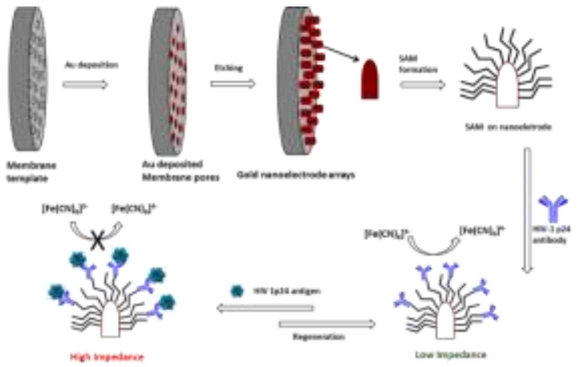

Fig.1 Schematic illustration of the different steps for the immunosensor construction

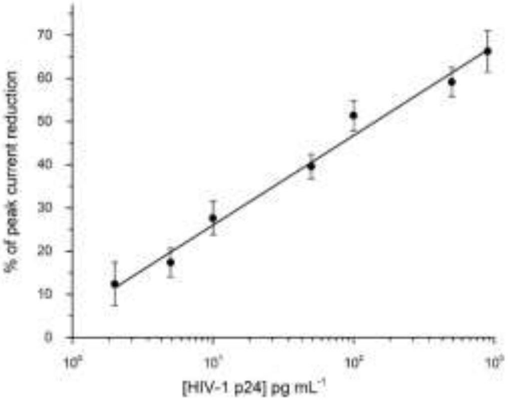

Fig.2 Calibration plot for the immunosensor

Key words: biosensor, HIV, biomarker, nanoelectrode, electrochemical sensor,

2.12 Molecularly imprinted polymer-based electrochemical sensor for MTB Biomarker

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A molecularly imprinted polymer-based electrochemical sensor for detecting early secretory antigenic target 6 (ESAT6) in blood serum samples was developed. Gold nanoelectrode ensembles (GNE) were prepared by electroless deposition of the gold within the 50 nm pores of polycarbonate particle track-etched membranes. A simple controlled solvent etching procedure based on the solubility of polycarbonate membranes in solvent mixtures is adopted to fabricate the GNE. Gold nanoelectrode was used to attain good conductive support for the electro-polymerization of the molecularly imprinted electrodes. Density functional theory (DFT) at B3LYP/6-31+G (d,p) level was used to calculate the molecular-level interaction between selected target MTB biomarker ESAT6 proteins and MIP. The pyrrole and 3-thiopheneacetic acid are electrochemically polymerized in the presence of a template biomarker molecule (ESAT6) on the electrode surface. Biomarker protein imprinted cavities were formed by removing entrapped biomarker molecules from the polymer film. Under optimal conditions, the developed sensor showed reasonable increments at the studied concentration range of 1–100 ng mL−1 for ESAT6. The lowest detection limit was found to be 0.5 ng mL−1 for ESAT6. Spiked human blood serum samples were analysed. The presence of non-specific proteins in the serum did not significantly affect the sensitivity. Molecular imprinting using synthetic polymers and nanomaterials provides an alternative approach to the trace detection of biomarker proteins.

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2.13 Molecularly imprinted polymer-based Electrochemical sensor for Aflatoxin B1

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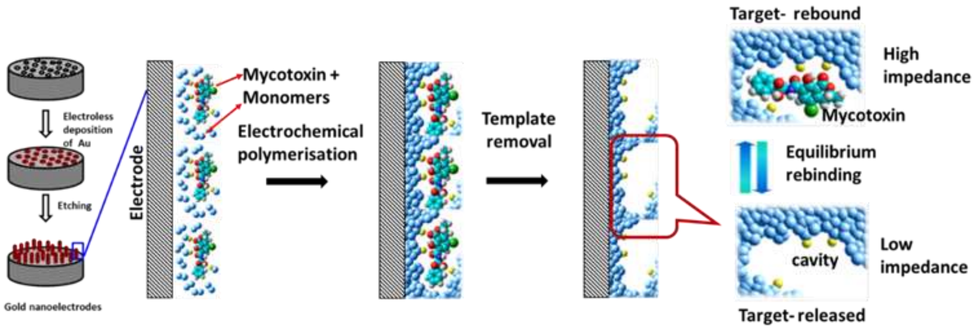
In the humid monsoon tropical climate of southern India, rice is one of the most important crops. The protection against crop damage caused by fusarium and Aspergillus species is essential. Aflatoxin B1 (AFB1) is considered the most toxic and is produced by both Aspergillus flavus and Aspergillus parasiticus. Aflatoxins have caused much harm to human and animal health due to their toxicity and carcinogenicity. It is estimated that about 4.5 billion people are chronically exposed to Aflatoxins. Since it is impossible to reverse its carcinogenic effects, the identification and prevention of human exposure to aflatoxins have become a major research topic in food science. Therefore, effective detection of AFB1 in food products is indispensable for ensuring that the products offered to meet regulatory and market requirements. A molecularly imprinted polymer-based electrochemical sensor for detecting AFB1 in rice samples was developed. Gold nanoelectrode ensembles (GNE) were prepared by electroless deposition of the gold within the 50 nm pores of polycarbonate particle track-etched membranes. A simple controlled solvent etching procedure based on the solubility of polycarbonate membranes in solvent mixtures is adopted to fabricate the GNE. Gold nanoelectrode was used to attain good conductive support for electro-polymerising the molecularly imprinted electrodes. Density functional theory (DFT) at B3LYP/6-31+G (d,p) level was used to calculate the molecular-level interaction between selected target AFB1 and MIP. The pyrrole and 3-thiophene acetic acid are electrochemically polymerised in the presence of a template molecule AFB1 on the electrode surface. AFB1 imprinted cavities were formed by removing entrapped AFB1 molecules from the polymer film. Under optimised experimental conditions, DPV was recorded for various concentrations of AFB1. The reliable capacity of the prepared MIP sensor was monitored by 30 min incubation at pH 7.4. The response of the MIP electrode to AFB1 was found to increase with increasing analyte concentration. A linear calibration graph was obtained in the general concentration range of 5-50 ng mL-1. The calibration graph plotted between the logarithm of AFB1 concentration and the peak current results with a correlation coefficient of 0.97. LOD is found to be five ng mL-1. Molecular imprinting using synthetic polymers and nanomaterials provides an alternative approach to the trace detection of AFB1.



Scheme 1. Schematic representation of MIP sensor for Aflatoxin B1 fabrication and sensing mechanism.

Key words: Imprinted polymer, Aflatoxin B1, electrochemical sensor, mycotoxin

2.14 Ion-Selective Organic Electrochemical Transistors Fabrication and testing

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Organic electrochemical Transistors (OECT) are used as transducers in biochemical sensors due to their sensitivity, ease of fabrication and compatibility in aqueous medium. It is generally described as a thin film transistor that couples an electronic and an ionic circuit. An OECT is typically made of three electrodes, source (S), drain (D), and gate (G). The conductance of the conducting polymer channel, that connects S and D, is modulated by the potential applied to gate (V G). In this work, a simple OECT was fabricated using conducting polymer thin film. Gold electrodes were deposited on thermally grown 300 nm SiO 2 on Si substrates by e-beam evaporation using a shadow mask. The conducting ink consisting of PEDOT: PSS and 1 wt % Dimethylformamide is coated by doctor's blade method followed by drying at 70 ^{0}C. The I-V characteristic of the device follows the Bernard-Malliaras equation indicating the conventional behaviour. The pinch-off potential, hole-mobility and transconductance of the device were 0.99 V, 1.7×10 3 m/Vs and 2.48×10 -4 S (at V G = 0.6 V), respectively. Its low operational potential and moderate transconductance make it suitable for biosensing application. After initial characterization of the OECT, it takes for further device performance analyses using different electrolytes, The anion of the electrolyte chose sulfonate and cation of the material took hydrogen and alkali material. The different cationic electrolytes are 50 mM of H2SO4, Li2SO4, Na2SO4, and K2SO4 taken, size of cation plays the key role in drain-source resistivity. The larger size of the cation decrease holes mobility in the channel then smaller one, Increase in cation size, decrease the oxidation state of PEDOT or in other words larger size of cation at the same potential penetrate the channel in high ratio and more cations doped with PSS than smaller one.

Keywords: Organic electrochemical transistor, conducting polymer, biosensor, dielectric.

2.15 Molecularly Imprinted Polymer Electrochemical Sensor for Capecitabine

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An anticancer drug capecitabine based chemotherapy for the stomach, breast and other cancers is well-known. Capecitabine detection in the human body is crucial since its high levels can have a variety of negative repercussions, including allergic problems, blood clotting issues, heart problems, and others. So, its measurement is essential. To study

the level of capecitabine, a novel electrochemical sensor was created using the molecular imprinting process. In this technique, electrochemically polymerises pyrrole using cyclic voltammetry (CV) in an Electrochemical workstation on a glassy carbon electrode (GCE) with capecitabine as a template molecule. By releasing capecitabine molecules from the polypyrrole film's entrapment, capecitabine imprinted cavities were created. By using the differential pulse voltammetry (DPV) technique, the capecitabine concentration in both reference and real samples was determined using the MIP electrode. MIP performance exhibits superior results when compared to NIP Electrode. When compared to other analytical techniques like High performance liquid chromatography (HPLC) and HPLC-mass spectroscopy, it is a cheap and simple way to find capecitabine concentration. Additionally, the molecular imprinting polymer method of sensing exhibits specificity and selectivity for capecitabine detection.

Keywords: Capecitabine, Electrochemical sensor, Molecular imprinting polymer, Polypyrrole.

2.16 Synthesis of Nanostructured gC_3N_4 composite and its Electrochemical sensing application.

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Nanocomposite with heterostructured nanomaterials was conferred for superior physiochemical properties. Herein, MoO3/gC3N4 nanocomposite was synthesized via hydrothermal method which is proposed to exhibit superior electrochemical sensing of biomolecules. Graphitic Carbon Nitride (gC3N4) is a semiconductor which drawn lots of attention due to its strong oxidative ability, high thermal and chemical stability, minimal cost of production, and its non-toxicity. Instead of the C-C bond in graphene, incorporating some heteroatoms like nitrogen into carbon-based materials enhances the properties of the existing material. Due to the lone pair present in the nitrogen, it acts as an electron donor site and promotes better catalytic conductivity, and endows tri-s-triazine tectonic units with unique electronic structures. Molybdenum trioxide (MoO_3) is

a promising semiconductor that has applications in energy storage, superconductors, gas and biomedical sensors. It has variable oxidation states which promote better catalytic activity. It is chemically stable, has better biocompatibility, and has excellent electrical and surface charge properties. Due to its polar nature and variable oxidation states it facilitates better binding of biomolecules and faster electron transfer leads to improved sensitivity. Combining Molybdenum trioxide with a 2D-Carbanaceous material (gC3N4) results in increased electron and ionic mobility with enhanced chemical kinetics.

Keywords: gC_3N_4, heterostructure, synergistic effects, electrochemical sensing.

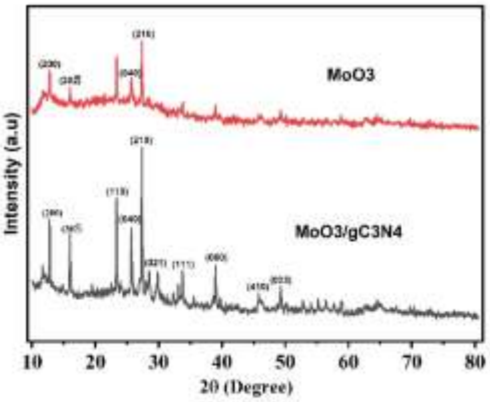

Fig. XRD patterns of MoO3 and MoO3/gC3N4

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2.17 Ru modified ZnO/rGO interface for engineering flat sheet like structure for ammonia gas sensing at room temperature

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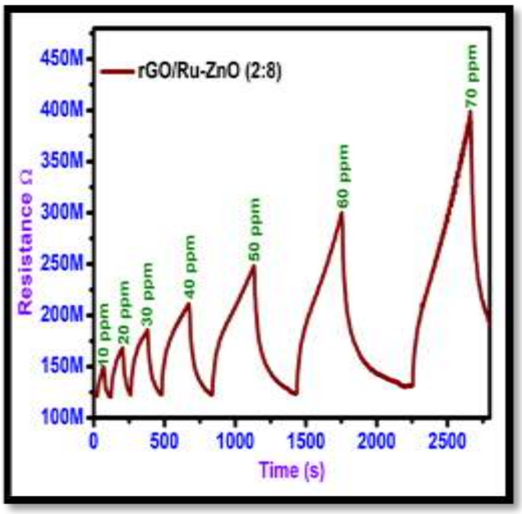
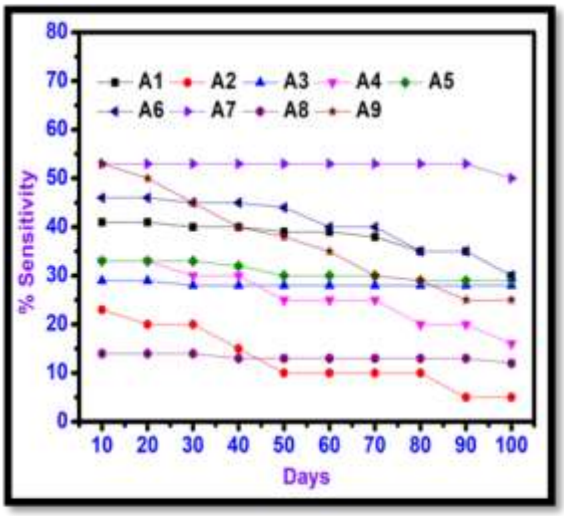
Creating a better surface activeness in a composite nanomaterial remains challenge for the researchers due to mismatching of appropriate material combinations. Individual properties of the materials play a vital role in increasing or decreasing the potentials of applications. Room temperature operative gas sensing electrodes with long term stability and highly selective feature are crucial to meet the miniaturization of gas

sensing devices. Ammonia (NH3) is an irritant gas consists of pungent odor in nature. Here, we report a synthesis method for the composite of Ruthenium nanoparticles modified Zinc oxide - reduced graphene oxide for NH3 sensing via two step sonication assisted hydrothermal method. The physiochemical and morphological characterization were examined well in detail. The results indicate the high crystalline Ru nanoparticles were assembled over the rGO sheets in a regular manner. The chemically active defect sites on the rGO sheets enhance the gas molecule adsorption and provide high electrical conductivity. This sensing electrode was exposed towards various target gases and it offered excellent selectivity and good sensitivity of 53 % towards 50 ppm of NH3 with response time 25 s and recovery time 34 s. In addition, this electrode maintains 90 % of its initial sensitivity after 100 days which proves its high stability due to the room temperature operation. This prepared composite material will be a good candidate against NH3 detection.





2.18 Synthesis and Characterization of Oxalic Acid (Oxa)-Induced Cobalt (Co) And Nickel (Ni) Bimetallic Assembled Polyaniline (Pani) Nanocomposite for Electrochemical Detection Of L-Tyrosine

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Here, we have synthesized an oxalic acid (Oxa)-induced cobalt (Co) and nickel (Ni) bimetallic assembled polyaniline (PANi) nanocomposite as a bifunctional material through a microwave-assisted method where the Oxa was used as a complexing agent to determine the final particle size distribution of the metal dispersion. The as-prepared materials were characterized well using FTIR, XRD, SEM and XPS. Among the prepared Co–Oxa, Ni–Oxa, Co–Oxa–Ni and Co–Oxa–Ni@PANi electrode materials, Co–Oxa–Ni@PANi nanocomposite employed as a sensitive electrochemical L-tyrosine (L-Tyr) sensor. L-Tyr is one of the several amino acids that contribute to re-growing healthy hair. Too little of this hormone causes stress-induced hair loss High level of tyrosine also causes liver and kidney failure, softening and weakening of the bones (rickets), and an increased risk of liver cancer (hepatocellular carcinoma). Hence the detection of tyrosine is must and Co–Oxa–Ni@PANi shows high sensitivity towards L-Tyr.

Keywords: Bifunctional material, amino acid and electrochemical sensor.

2.19 A biomimetic sensor for electrochemical detection of salivary nitrite levels

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The nitrate-nitrite-nitric oxide pathway plays crucial role in regulating blood flow, metabolism, cell signaling and protecting tissues from oxidative stress induced cell damage. The levels of nitrite (NO2-) in human saliva are correlated to the circulating nitric oxide (NO) and used as predictive biomarker to assess endothelial function. Nitrate (NO3-) in plasma is secreted into saliva and reduced to NO2- by salivary nitrate reductase enzyme. Thus, the measurement of NO2- in saliva will be useful in the fields of cell biology and biomedical analysis. A number of methods such as capillary electrophoresis, spectrophotometry, chemiluminescence and chromatography have been widely used to measure NO2- levels. Although the methods provide many advantages, the conventional procedures have certain limitations, which includes time consumption, susceptibility to ionic interference and requiring expensive equipment. In contrast to these methods, we attempted to develop a simple direct approach for measuring NO2- levels in human saliva by selective reduction to nitric oxide (NO). In this study, a low-cost electrochemical sensor platform is developed using screen-printed carbon electrodes (SPCE). For selective measurement of NO2-, biomimetic catalysts involving bioinorganic macromolecules such as porphyrins and chlorphyllins were integrated onto multi-walled carbon nanotubes (MWCNTs) modified electrodes. The electrochemical sensors showed good electrocatalytic activity towards the oxidation and detection of NO2- levels in in human saliva. The porphyrin-based electrochemical sensor showed good a wide linear range of response for NO2- in the concentrations ranging from 10 µM to 5 mM with a detection limit of 1 µM. The performance of the proposed sensor is also tested in measuring the NO2- levels in human saliva samples.

2.20 Development of An Electrochemical Sensor based on a Manganese Cobalt Oxide Nanoparticle for Detection of Antipsychotic Drug

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In this study, we have demonstrated a simple and more accurate electrochemical sensor. As-prepared Binary transition metal oxides nanoparticle (BTMOs) $MnCo_2O_4$ (MCO) is drop cast on the glassy carbon electrode and its electro catalytic performance is analysed for Olanzapine. Herein, (MCO) nanoparticle was synthesized by simple co-precipitation process using sodium hydroxide as a precipitating agent and subsequent elimination by calcination. The structural and morphological study was examined by various methods, including UV, FT-IR, and XRD analysis. The electrochemical activity of the fabricated electrode has been optimized through varying pH, loading quantity, and scan rates. The electrochemical characteristics were performed by CV, EIS, DPV, and Amperometric (i-t) techniques. Under optimized voltammetric conditions, the as-proposed sensor shows good performance towards oxidation potential with a linear range.

Keywords: Binary transition metal oxides, Differential pulse voltammetry, antipsychotic drug.

2.21 Structural elucidation and spectroscopic studies of acetyl substituted piperazine nucleus tethered with 4, 5-diaryl-1 H-imidazole scaffold: DNA binding, $Cu^{2+}$and Sn^{2+} ions sensing and cytotoxicity

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In this study, we report synthesis of new imidazole based fluorescent chemosensors2-((4-(5-bromo-2-hydroxy-3-(4,5-diphenyl-1H-imidazol-2-yl)benzyl)piperazine-1-yl)methyl)-4-bromo-6-(4,5-diphenyl-1H-imidazole-2-yl)phenol(1)and2-((4-(2-hydroxy-5-methyl-3-(4,5-diphenyl-1H-imidazol-2-yl)piperazine-1-yl)methyl)-4-methyl-6-(4,5-diphenyl-1H-imidazole-2-yl)phenol(2). The synthesized chemosensors1 and 2 were characterized by FT-IR, 1H NMR, UV-visible andfluorescence spectral studies. Further, the single crystal X-ray diffraction analysis shows that the chemosensor1crystallizes in triclinic system, with space group P-1.Hirshfeldsurface analysis and 2D fingerprint maps revealed that 1have remarkable H...H, C...H/H...C, and O...H/H...O Br...H/H...Br, interactions. The chemosensorswere developed for selective and sensitive detection of Sn2+ and Cu2+ions in methanol among other tested cations. Both chemosensors1 and 2exhibits “turn-off” fluorescence response to Cu2+ and “turn-on” fluorescence enhancement to Sn2+ ions. Moreover, the fluorescence imaging in A549 cells suggested that chemosensors had great potential in the application of bio-imaging. The chemosensors1 and 2 with Sn2+ ions were found to be cytotoxic against A549 cells and could be used as an anticancer agent.

Keywords: Chemosensor, Imidazole, Sn^{2+} and Cu^{2+} ions, DNA binding studies, Bioimaging, A549 cell.

2.22 Hydrothermal-Assisted Synthesis of Strontium Cerate Nanoparticles ($SrCeO_3$ Nps) for the Selective Electrochemical Detection of Dopamine

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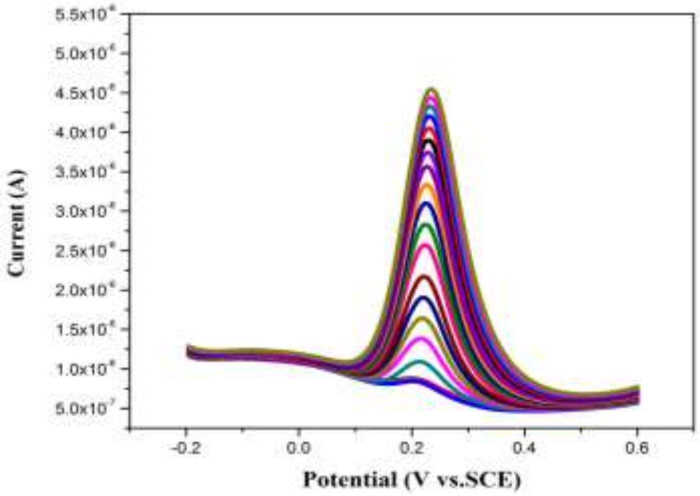
In this work, we have demonstrated the preparation of Strontium Cerate Nanoparticles ($SrCeO_3$ Nps) for the Selective Electrochemical Detection of Dopamine via simple hydrothermal method. The structural and morphological properties were characterized by XRD, FT-IR, XPS, SEM and TEM. The electrochemical characteristics were performed by CV, DPV, and amperometric (i-t) techniques. $SrCeO_3$/GCE shows more enhanced electron transport property, higher surface area and more efficient electrocatalytic activity towards Dopamine. It is expected that $SrCeO_3$/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of Dopamine.



Keywords : Strontium Cerate, nanoparticle, sensitive, detection and dopamine.

2.23 A selective and reversible "Off-On" Rhodamine B derivative with β-cyclodextrin inclusion complex fluorescent chemosensor for dual metal ions recognition

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Herein, design and synthesized the fluorescence probe of syringaldehyde-based rhodamine derivative of ((E)-3',6'-bis(diethylamino)-2-((4-hydroxy-3,5-dimethoxy benzylidene) amino) spiro[isoindoline-1,9'-xanthen]-3-one (RhSy). The synthesized molecule structure, functional group, and molecular mass were determined and characterized by 1H-NMR, FT-IR, and Mass-spectroscopy techniques. Additionally, it has been entrapped within β-Cyclodextrin (RhSy@β-CD) through supramolecular assembly to enhance solubility and stability. The binding constant between RhSy and β-CD is determined using the Benasi-Hildebrand equation. The RhSy & RhSy@β-CD acts as a fluorescence probe for the detection of copper (Cu2+) and Ferrous (Fe3+) ions in a CH3CN/H2O (9:1) medium. The naked eye observation is more appropriate than other spectroscopic techniques. Increasing the concentration level of Cu2+ and Fe3+ remarkable change from colorless to dark pink. A drastic change in the fluorescence result, the addition of Cu2+ and Fe3+ into the RhSy probe, and the emission intensities have enhanced (in the 526 nm range). A linear correlation when plotting the increasing concentration of Cu2+ and Fe3+ versus emission intensities. The fluorescent confocal studies also support the "off-on" mechanism.

Keywords: Rhodamine derivative, absorption intensity, emission property, sensing, Cu^{2+} *and* Fe^{3+}

2.24 Fabrication of Dysprosium Molybdate-Aloe Vera Activated Carbon Nanocomposite for Electrochemical Determination of Vanillin

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For the first time, we are successful in the synthesis of structurally specific Dysprosium Molybdate-Aloe vera Nanocomposite using hydrothermal followed by calcination method. The structural and morphological properties were characterized by X-ray Diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), Raman Spectroscopy, X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). The electrochemical characteristics were performed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS)

differential pulse voltammetry (DPV), and amperometric (i-t) techniques. Dysprosium Molybdate-Aloe vera/GCE shows more enhanced electron transport property, higher surface area and more efficient electrocatalytic activity towards Vanillin. It is expected that Dysprosium Molybdate-Aloe vera/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of Vanillin.

Keywords: Dysprosium Molybdate, Aloe vera, Hydrothermal method, Biosensors and Vanillin.

2.25 Ferrocene-Based Receptor for Sensing Cation/Anion studied for its Biological Activities

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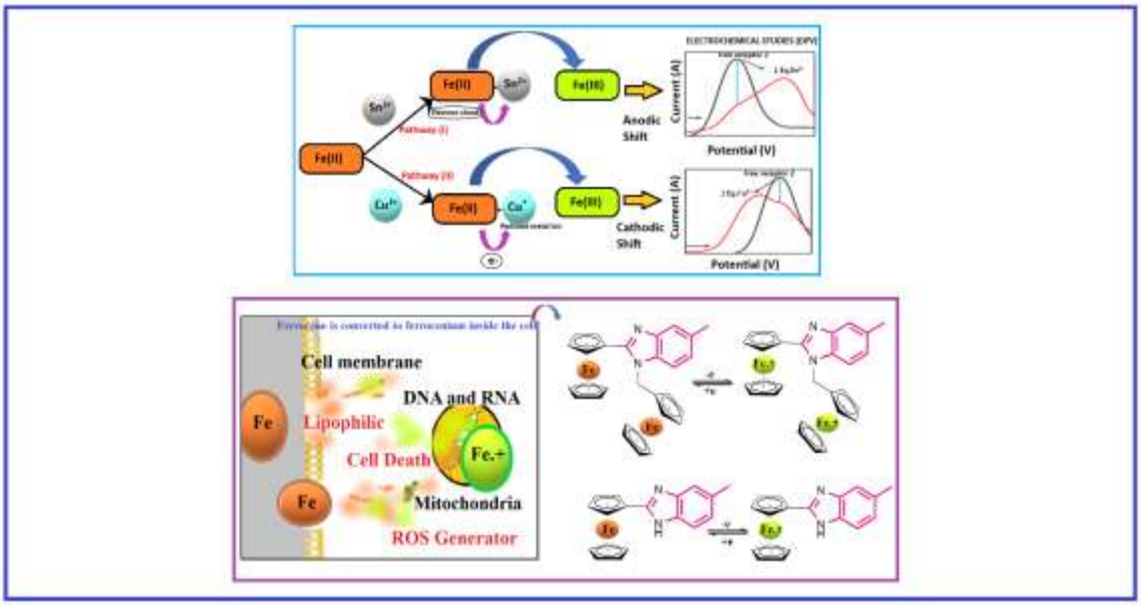
The newly synthesized ferrocene conjugated 5-methylbenzimidazole, compound 1 bearing di- ferrocene and compound 2 having mono ferrocene were obtained by intramolecular cyclization of 3, 4 diamino toluene with ferrocene carbaldehyde resulting in minor and major products 1 and 2 respectively (where 1 = 1-(ferrocenylmethyl)-2-ferrocenyl-5-methyl-1H-benzo[d]imidazole and 2 = 2-ferrocenyl-5-methyl-1H-benzo[d]imidazole). The ferrocene based molecules 1 and 2 were characterized by FT-IR, NMR (1H, 13C, and DEPT), elemental analysis and ESI Mass spectral analysis. The optical and electrochemical studies confirm the sensing of cations and anions with excellent selectivity and sensitivity towards Sn2+ by receptor 1 and Sn2+/Cu2+ by receptor 2. The binding constant (Kb) was calculated for receptor 1 as 1.28 x 102 M-1 (Sn2+) and receptor 2 as 3.2 x 103 (Sn2+), 2.68 x 102 (Cu2+) and 4.46 M-1 (F-) respectively. Further, receptor 1 lacks hydrogen bonding and hence shows no anion sensing, whereas receptor 2 having selective sensing of F- ion via electrostatic communication shows a 1:1 complexation in the Jobs plot. The biological activity for receptors 1 and 2 was studied against a Gram-positive (S. aureus), a Gram-negative (E. coli), and a fungi strain (C. albicans). The zone of inhibition, MIC, and MFC results show that receptor 1 has significant fungal activity than receptor 2 and standard drug. The cytotoxicity observed for receptors 1 and 2 was moderate when evaluated against the liver cancer cell line (HepG2) by MTT method, the IC50 value obtained was 32.27 µM and 41.43 µM for receptor 1 and 2 respectively, hence receptor 1 having two ferrocenes is more cytotoxic than receptor 2.

Key words: Ferrocene based receptor, optical sensing, electrochemical sensing, anti-microbial and anti-cancer.

Graphical Abstract



2.26 Oxalamide-Bridged Imidazole based 'Turn Off' Fluorescent Receptor for Cu^{2+} and Fe^{3+} ions

Parvathavarthini Murugaperumal[1], Priyanga Kalimuthu [1],Saroth Nafila Niyazudheen[1], Sengottuvelan Nallathambi[2]

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We describe the synthesis of symmetrical N, N'-bis(3-(1H-imidazol-1-yl) propyl) oxalamide based receptor OX(PID)2 and characterized by different physico-chemical techniques via FTIR, 1H-NMR, 13C-NMR, TGA and mass spectrometry. The single crystal X-ray diffraction analysis shows that the OX(PID)2 crystallizes in monoclinic, with space group P 21/c. The sensing capability of OX(PID)2 towards various cations has been exhaustively investigated using UV-vis and fluorescence spectroscopy. The OX(PID)2 shows high selectivity and sensitivity towards Cu2+ and Fe3+ ions with 1:1 binding ratio to over other metal ions and which was highly supported via Job’s plot and density functional theoretical calculations. The Cu2+ and Fe3+ ions are inducing the ‘Turn-Off’ signal when interaction with OX(PID)2. Moreover, the fluorescence imaging in A549 cells on receptor OX(PID)2 suggested that OX(PID)2 had great potential in the application of bioimaging. The receptor with Cu2+ or Fe3+ ions were found to be cytotoxic against A549 cells and could be used as an anticancer agent.

Keywords: Oxalamide, Single crystal X-ray diffraction, Copper ion, Iron (III) ion, A549 cells,

2.27 Ultrasonic-Assisted Synthesis of Praseodymium Molybdate Nanoparticles for the Selective and Sensitive Electrochemical Detection of Antagonist drug

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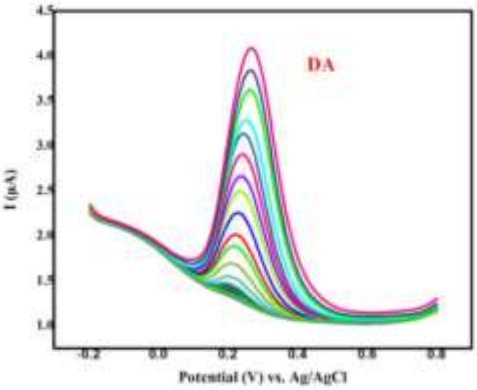
In this work, we have developed the synthesis of Praseodymium Molybdate nanoparticles for the selective and sensitive electrochemical detection of antagonist Drug. Dopamine (DA) is a type of monoamine neurotransmitter, also known as “Feel – good” hormone. The abnormal levels of DA causes certain physiological problems. So, here we developed a sensitive electrochemical sensor for a detecting the Dopamine based on a glassy carbon electrode (GCE) that was modified with a Praseodymium molybdate (PM) nanoparticles. The synthesized Praseodymium molybdate nanoparticles was examined by UV, FT-IR and XRD and the electrochemical studies are discussed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV) and amperometry. Praseodymium molybdate/GCE shows more enhanced electron transport property, higher surface area and more efficient electrocatalytic activity towards Dopamine. It is expected that Praseodymium molybdate/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of Dopamine.



Keywords: Praseodymium molybdate, ultrasonication, neurotransmitter and antagonist drug.

2.28 Synthesis of nanostructure graphene composite and its electrochemical sensing application

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Metal oxides play an important role in the fabrication of electrochemical sensors. Electrochemical sensors using metal oxide facilitates redox and catalytic activity such that the selectivity, sensitivity and cycling stability is achieved. In this present work, cerium oxide (CeO_2) can show a number of properties, such as catalytic activity, biocompatibility, strong conductivity, a large surface area, and the capacity to transport oxygen, that have drawn a lot of interest in the development of very sensitive biosensors. Aside from CeO2, the combination of graphene's appealing properties with the excellent properties of other functional nanomaterials has become a popular path for achieving applications in a variety of fields. Herein, reduced graphene oxide (rGO) is a single-layer sheet that is two-dimensional (2D) and has great physico-chemical characteristics for good conductivity and functionality. By adding both rGO-CeO_2 nanocomposites, which are synthesised using a simple one-step hydrothermal treatment to form rGO nanocomposites with CeO_2, they were able to increase the concentration of oxygen vacancies coupled with rGO, resulting in faster charge transfer, which can further improve their performance rGO-CeO_2. It also appears that the crystal structure of the CeO_2 nanoparticles has a significant impact on the sensing ability of rGO-CeO_2 composites, with the regular hexagonal nanocrystal CeO_2 having the highest sensitivity. The nanocomposite achieves rapid electron transfer when combined with metal oxide, making it a useful and effective electrochemical sensor that can further boost the productivity of electrochemical sensors.

Keywords: Electrochemical sensors, Metal oxide, Hexagonal crystal, Sensitivity.

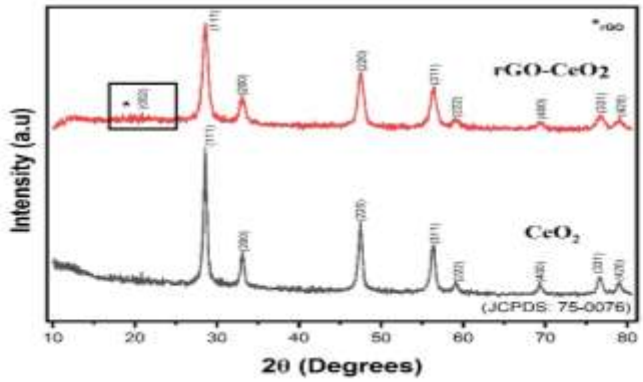

Fig. XRD Pattern of CeO_2, rGO-CeO_2.

Reference :

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2. S. Ansari et al. / Materials Today: Proceedings 18 (2019) 1210–1219.

2.29 Investigation Of The Electrocatalytic Activity Of Bismuth Molybdate Nanoparticle For The Voltammetry Determination Of Ascorbic Acid

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In this work, we developed a Bismuth molybdate nanoparticle for electrochemical detection of Ascorbic acid (AA). The formation of the Bismuth molybdate nanoparticle was systematically examined by X-ray Diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), Raman Spectroscopy, X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). The electrochemical characteristics were performed by cyclic voltammetry (CV),

electrochemical impedance spectroscopy (EIS) differential pulse voltammetry (DPV), and amperometric (i-t) techniques. The Bismuth molybdate modified GCE exhibit a high electrocatalytic performance toward AA detection comparable to bare GCE. The excellent electrocatalytic activity of the Bismuth molybdate nanoparticle can be attributed to its good conductivity, synergistic effect, and abundant active site.

Keywords: Bismuth molybdate, nanoparticle, electrocatalytic activity and ascorbic acid.

2.30 Synthesis of Schiff Base Ligand and its Metal Complexes and Application in Anion Sensing and Biological Activity

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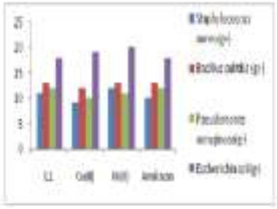
Two new metal complexes of Cu(II)) and Co(II) ions with a Schiff base derived from Substituted Salicylaldehyde and sulfadiazine have been synthesized and characterized by elemental analysis (C, N, O) and spectral (IR, UV, 1H NMR) studies. The coordination of the ligand to the metal ions is found to be through azomethine nitrogen and phenolic oxygen of the Schiff bases. In these complexes, the Schiff base acts as a bidentate ligand. Transition metal complexes derived from the Schiff base ligand with biological activity have been widely studied. The free ligand and their metal complexes have been screened for their in vitro biological activities against bacteria and fungi (Aspergillus niger, Candida albicans and Pencillium chrysogenum). The antibacterial activities of synthesized compounds were studied against gram positive bacteria: Staphylococcus aureus, Bacillus subtilis and gram negative bacteria: Pseudomonas aeruginosa and Escherichia coli by using the disc diffusion method. A comparative study of MIC values of the Schiff base ligand and their complexes indicates that the complexes exhibit higher antimicrobial activity than the free ligand. It is found that the metal complexes show more potent activities compared with Schiff base ligand. The anion sensor properties of the receptor Schiff base shows selective recognition towards F and CN anions over other anions. Appreciable color changes are observed when the receptor (L) is treated with

the fluoride and cyanide anions, imparting an immediate color change from colorless to deep yellow.



The molecular structure of Ligand, Minimum Inhibitory Concentration(MIC) values of ligand and the complexes

Keywords: Transition metal ions, Schiff base; Metal complexes; Antibiological activity

Reference:

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2.31 A new "naked eye" and "turn-on" fluorescent chemosensors: Schiff base azine derivative combined with γ-Cyclodextrin as a fluorescent probe for the detection of Fe^{3+} ions

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In recent years, the persistence of metal ions Fe3+ in the body of organisms causing potential hazards. Especially this metal ion is necessary for the normal homeostasis of organisms. The quantity level exceeding led to disorder. In this urgent situation, the detection of Fe3+ ions are more considering by an eco-friendly approach. To overcome this issue, the current study synthesis the water-soluble azine-based derivative of 4,4'-((1E,1'E)-hydrazine-1,2-diylidenebis(methanylylidene)) bis (2-methoxy phenol) commercially the name of Vanillin Azine (VAA) inclusion with γ-Cyclodextrin (γ-CD) (γ-CD/VAA) probe for the detection of Fe3+ ions. The structural, functional, and optical properties of VAA and γ-CD/VAA were characterizing by 1H NMR, 2-D NMR (ROESY), FT-IR, and UV spectroscopy. Which probe is very sensitive and selective (detect the ions at nano level) and targeted fluorescence-enhancing response to Fe3+. The limit of detection (LOD) and binding constant values of γ-CD/VAA with Fe3+ calculated through the absorption, and fluorescence titration method. To exact binding sites of the probe with Fe3+ ions are theoretically explained using a DFT study in B3LYP function in PM3 calculation mode. The "turn-on" fluorescence confirmed by confocal fluorescence imaging, and the probe's biocompatibility formulates the MTT assay live cell imaging. Additionally, the molecular mass of the γ-CD/VAA/ Fe3+ identified by HR-Mass spectroscopy. Overall, this study proved that a minimal quantity of Fe3+ ions in the biota and natural sources have detected (γ-CD/VAA).

Keywords: Vanillin Azine, γ-Cyclodextrin, Fe3+ions, fluorescence, turn-on.

2.32 Hydrothermal synthesis of Dysprosium Molybdate employed for the Electrochemical sensing of Uric acid

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In this work, we have demonstrated the preparation of Dysprosium Molybdate employed for the Electrochemical sensing of Uric acid via simple hydrothermal approach. The structural and morphological properties were characterized by X-ray Diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM) and Transmission electron microscopy (TEM). The electrochemical characteristics were performed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV), and amperometric (i-t) techniques. Dysprosium Molybdate/GCE shows more enhanced electron transport property, higher surface area and more efficient electrocatalytic activity towards Uric acid. This nanoparticle has been utilized as an electrode modifier for the electro-oxidation of uric acid. Furthermore, it has been

found to show the enhancement in peak current and shift of the oxidation potential in a negative direction by comparison to bare GCE. Due to the higher surface area, higher stability, improved electrocatalytic activity towards the detection of uric acid with a low detection limit (0.3811 uM) and higher sensitivity (4.615 uA µM-1 cm2) were achieved. It is expected that Dysprosium Molybdate/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of Uric acid.

Keywords : Dysprosium Molybdate, Hydrothermal synthesis, Electrochemical sensor, Uric acid.

2.33 Active sites tailored rGO nanosheets with high crystalline metal oxides nanocrystals for ammonia e-sensitization at room temperature

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Metal oxide gas sensors are an efficient and cost-effective way to protect our lives and property from accidental incidents. They are arguably the safest type of gas sensor, as they detect only a limited range of gases. They also require very little maintenance or calibration, which makes them perfect for numerous applications. However, traditional devices cannot meet the needs of our fast-developing mobile society because they have high operating temperatures and are unsuitable for battery-powered portable systems that can only drive devices with low power consumption. In this present work, we demonstrated room-temperature gas sensing properties of reduced graphene oxide and polypyrrole layers with different temperature calcined SnO_2 deposition through a facile polymerization and hydrothermal method. Apart from the physiochemical characterizations, the material was also used for analyzing the electrochemical behavior using cyclic voltammetry and impedance analysis. This nanocomposite of the rGO-PPy-600 SnO_2 electrode shows the highest sensitivity for a 10-ppm concentration of ammonia. This enhanced sensing behavior was caused by electronic sensitization between the surface p-n heterojunctions between layers and metal oxides. The electrode withstands long-term stability of 88 % for 50 days. This simple and inexpensive

technique will be a possible contender for making ammonia gas sensors that can operate at room temperature.

Keywords: gas sensor, p-n junction, SnO2 nanoparticles, hydrothermal, polypyrrole.

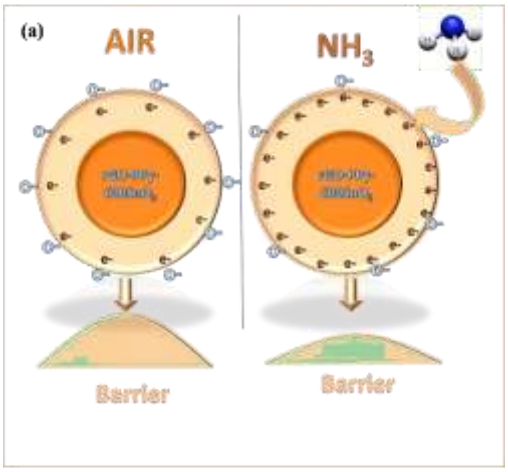

Fig. Schematic of gas sensing mechanism

Reference : A. Alengebawy, S. T. Abdelkhalek, S. R. Qureshi, and M.-Q. Wang, “Heavy metals and pesticides toxicity in agricultural soil and plants: Ecological risks and human health implications,” Toxics, vol. 9, no. 3, p. 42, 2021.

2.34 Fabrication of Screen-Printed Carbon Electrode Integrated with Paper-Based Microfluidic Platform for Sensor Applications

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The nineteenth century could see the advent of screen printing as a method of industrial scale production. Currently, screen printing is a well-respected and widely used method for creating printed circuits and electrodes. Screen-printed electrodes (SPEs) are mass-produced, inexpensive, disposable electrochemical devices. Making screen-printed electrodes is made easy, beautiful, and versatile by using screen printing. Capacitors, resistors, and conductors are manufactured using highly developed screen-printing techniques and materials on alumina substrates for use in hybrid electronic circuits.

Moreover, there are formulations for printing on plastic, steel, and glass substrates to create electrical components and aesthetic patterns. components needed to make screen-printed electrodes A manual screen-printing machine, printing mesh, printing dies, a UV lamp, and ink are all present. Different types of ink, including graphite ink, are examined in order to get the right consistency of ink for making screen-printed electrodes. The paper serves as the support substrate for the electrodes and the composite where sample and recognition bio-molecules are combined and react in paper-based electrochemical biosensors. Microfluidic channel integrated with a screen-printed electrode that passes through paper Model redox indicators were used to test the electrode assembly. Thick-film chemical or biological sensors are always being improved due to this study. The focus of evolution is on how to make biosensor strips for tiny portable devices that allow monitoring of various species of interest, such as glucose and other clinically significant substances, or contaminants, such as pesticides.

Keywords: screen-printed electrodes, paper-based sensor, biosensors

3. Computational Chemistry

3.1 Study on In silico Molecular Docking and Molecular Dynamic Simulation of Computationally Designed twin drug against Breast Cancer

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Breast cancer is one of the second leading causes of death in women worldwide. There are many types of treatment for breast cancer such as surgery, radiation therapy, and chemotherapy. Chemotherapy drug is the best option for the patient's choice of treatment. Due to have several disadvantages the existing drugs are not effective. In order to avoid the drawbacks, new with novel and effective drug are to be needed. In this present study, we designed the twin drug (CLA-DSP-CLA) using Cladribine (CLA) as hydrophobic anticancer drug with linker. Dithiobis(succinimidyl propionate) (DSP) using computational approach. The designed twin drug and native drug was subjected to Molecular Docking, Binding Free Energy, and ADME prediction using Schrodinger software. Further Molecular Dynamic Simulation was performed by GROMACS software. The designed twin drug (CLA-DSP-CLA) has shown good highest docking score (−8.97 kcal/mol) with four H-Bond interaction, better binding affinity, admirable stability and acceptable Pharmacokinetics properties when compared to native drug. Therefore, the designed twin drug could be considered good leads for further preclinical and clinical experimentations as potentially efficient anticancer agent against breast cancer.

Keywords: Breast Cancer, Molecular docking, Molecular dynamics simulation, Pharmacokinetics properties, twin drug.

Acknowledgments

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3.2 Computationally designing Glutathione-CeO_2 anticancer Agent for Drug Discovery against Breast Cancer Treatment

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Breast Cancer is second leading cause of disease related death. The CDK is plays a vital role in the regulation of the cell division and over expression of CDK12 which leads to cause the cellular aberrations of cancer. Several active targeted molecules such as small molecules and antibodies have been identified. Due to have low drug delivery along with severe side effects, the active targeted molecules are not suitable against breast cancer. Appropriate targeting is one of the key issues in the development of anticancer drug, requiring that the anticancer drug reaches the targeted area and efficiently induces its pharmacological action without damaging healthy tissues. In this work, we designed a novel Glutathione-CeO_2 anticancer agent through Marvin Sketch. The designed anticancer agent was docked with CDK protein and it was subjected to the Molecular Dynamic Simulation (MDS) and ADMET properties. In the Molecular Docking analysis, Glutathione-CeO_2 anticancer agent has shown docking score is -48.34Kcal/mol. The MDS analysis reveals that the designed drug has maintained the constant stability throughout the simulation. The ADMET profiling shows that the Glutathione-CeO_2 has obeyed the drug likeness properties and it is not violated. Overall result suggested that Glutathione-CeO_2 anticancer agent could be used for breast cancer treatment.

Keywords: ADMET properties, Breast cancer, CDK12, Glutathione-CeO_2, Molecular Docking, Molecular Docking, Molecular Dynamic Simulation.

Acknowledgement: The authors thankfully acknowledge the UGC-Innovative [No. F.14-13/2013 (Inno/ASIST)], DST-FIST [SR/FST/LSI- 667/2016(C)], DST PURSE [SR/PURSE Phase 2/38 (G)], and MHRD-RUSA 2.0 [F.24/51/2014-U, Policy (TNMulti-Gen), Department of Education Government of India] and DBT- BIC [BT/PR40154/BTIS/137/34/2021] for financial support and infrastructure facilities. SM thanks the Indian Council of Medical Research (BMI/11(41)/2022 dated: 20.06.2022) for providing ICMR-SRF (Senior Research Fellowship).

3.3 In silico molecular docking and Molecular Dynamic Simulation of designed Drug-Drug Amphiphilic drug-drug against cancer

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Breast cancer is the most common type of cancer globally and its treatment with existing drugs manifests several limitations including poor bioavailability, inability to differentiate healthy and tumor cells, severe multidrug resistance, and adverse side effects to healthy tissues. To overcome the limitations, a new with novel and effective therapeutic agent are imperative. In this study, in silico approach was used to design novel the amphiphilic drug-drug conjugate against breast cancer treatment. Amphiphilic drug-drug conjugate was constructed by using two dissimilar drugs (Bendamustine and Topotecan) through the Marvin sketch. Then, Molecular Docking, Binding Free Energy and Molecular Dynamic Simulation were performed by using Schrodinger and GROMACS software. The results showed that the amphiphilic drug-drug conjugate has a better docking score (-9.676 Kcal/mol), and four hydrogen bond interactions. Moreover, the designed drug has shown good binding affinity (-56.358 Kcal/mol) and admirable stability during 50 ns simulation period when compared with native drugs. Furthermore, the amphiphilic drug-drug conjugate satisfied the drug-likeness properties which was studied from ADME prediction. From the analysis, it is concluded that the in silico approach may helps to develop a novel potent anti-cancer agent against breast cancer.

Keywords: Amphiphilic drug-drug conjugate, Breast Cancer, Molecular Docking, Molecular Dynamics Simulation, ADME prediction.

Acknowledgments

SM thanks the Indian Council of Medical Research (BMI/11(41)/2022 dated: 20.06.2022) for providing ICMR-SRF (Senior Research Fellowship). The authors thankfully acknowledge the UGC-Innovative [No. F.14-13/2013 (Inno/ASIST)], DST-FIST [SR/FST/LSI- 667/2016(C)], DST PURSE [SR/PURSE Phase 2/38 (G)], and MHRD-RUSA 2.0 [F.24/51/2014-U, Policy (TNMulti-Gen), Department of Education Government of India] for financial support and infrastructure facilities.

3.4 Computational study of BODIPY based donor molecules for organic solar cells application

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The precise design of organic photovoltaic material and the control of the band gap of the active layer are crucial for achieving high-performance organic solar cells (OSCs). The computational approach is a great tool to analyze the organic molecule's band gap nature and check the power efficiency behavior of OSCs. In this work, the BODIPY derivatives involved the DFT approach of Becke's three-parameter compound (B3LYP) for use as a donor in OSCs applications. We design fifteen BODIPY donor derivatives and filtered four efficient donor molecules Then, we studied the DFT and TD-DFT methods used to examine the photophysical properties, frontier molecular orbitals (FMOs), and density of states (DOS). The open circuit voltage (Voc) was also studied in which the BODIPY derivatives is a donor and the [6,6]-Phenyl C70 butyric acid methyl ester (PCBM) acceptor (A) is an acceptor. The work has demonstrated that D4 is best for solar cell application compared to others due to its excellent photovoltaic properties, which include the lowest bandgap (1.83 eV). As a result, the developed D1, D2, D3, and D4 molecules have excellent and outstanding performance that results suggesting the molecules are suitable donors for OSCs applications.

Keywords: DFT approach, BODIPY derivatives, band gap, organic solar cells.

3.5 Antioxidant activity and releasing behavior of vanillin from γ-cyclodextrin inclusion complex and electrospun nanofibers with polyvinyl alcohol; spectroscopic and computational studies

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Several active antimicrobial agent encapsulation strategies for food preservation based on the polymeric matrix have been improving in recent decades. This research looked at

the effectiveness of a Vanillin (VN) Inclusion Complex with γ-Cyclodextrin (γ-CD) for improving solubility and stability. It is also entrapping within polyvinyl alcohol (PVA) nanofibers (NFs), which offer outstanding nanosized, mechanical, thermal, optical, and textural qualities. The B3LYP/ 6-31G method has to be used to compute the four probability complex orientations (O-1, O-2, O-3, and O-4). The solid complexation was done through the co-precipitation process and the complex was characterized by FT-IR, XRD, H1-NMR, and 2-D H1-NMR (ROSEY). The binding constant can be evaluated by using absorbance, emission, and cyclic voltammetric experiments. We also make edible electrospinning NFs based on PVA/VN/γ-CD or PVA/VN in an aqueous medium. PVA is utilized as a stabilizing polymer to help the electrospinning solution. SEM and TGA analysis to determine the surface morphology, average fiber diameter, and improvement in thermal stability. The in-vitro (antibacterial, anti-oxidant, and dissolution NFs) effects of NFs on brine shrimp nauplii were also observed with the aid of spectrometric methods. Effects of NFs on brine shrimp nauplii that are harmful in vivo. Additionally, it is discovered to be a serious food issue in marine environments. Finally, our research suggests that produced NFs could be used in the food industry as food preservatives.

Keywords: Nanofibers, binding constant, cyclodextrin, anti-oxidant, food preservatives.

4. Electrochemistry

4.1 Inhibiting corrosion of Mg alloy AZ31 with Lithium based inhibitor

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The objective of the work is to determine the effectiveness of dissolved Lithium Carbonate as an inhibitor for magnesium AZ31 sheet metal when immersed in NaCl (aq) at ambient temperature. Inhibition of corrosion was investigated by Potentiodynamic polarization and Electrochemical Impedance Spectroscopy (EIS). The surface analytical measurements were done by X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM) and Energy Dispersion X-ray Spectroscopy (EDS). The manner in which inhibition is achieved is rationalized by the role played by the surface film produced during corrosion in inhibiting both the anode (anodic dissolution) and cathode (H2 Evolution) kinetics.

KEYWORDS: Corrosion inhibitor, Surface film, Magnesium, Lithium Salts.

4.2 Cobalt nickel sulfide Electrocatalyst for Oxygen Evaluation Reaction in alkaline medium

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Abstract

The development of a highly active, cost-effective, and sustainable electrocatalyst is highly essential for improving the sluggish kinetics of the oxygen evaluation reaction (OER) in the water splitting reaction. Especially, cobalt, nickel, and sulphide based spinel materials are auspicious candidates that significantly tune OER performance due to their improved catalytic active sites. In this work, we developed a cobalt nickel sulfide nanoparticles by using single step hydrothermal approach.

Subsequently, we altered the molarities of Co and Ni precursors, and the resulting CoNi2S4 materials were investigated for their electrochemical performance towards OER. Among them, the CoNi2S4-1 material demonstrated a highly crystalline nature, sponge like morphology, and higher concentration of Co content that significantly enhanced the octahedral Co3+ active centres, which greatly altered the electrochemical OER performance. Further, electrochemical results revealed that the CoNi2S4-1 material displayed better activity than that of benchmark RuO2 and had a potential of 1.819V vs. RHE for attaining a current density of 10 mA cm-2 in 0.1 M KOH electrolyte.

4.3 A Theoretical model of amperometric immobilized enzymes at three different geometry electrodes

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This article discusses the diffusion and kinetics of amperometrically immobilized enzymes on electrodes with three distinct geometries (planar, cylindrical, and spherical). A set of nonlinear reaction-diffusion equations with a non-linear term related to Michaelis-Menten kinetics and enzyme-catalyzed reactions are used to describe this model. By using the Akbari-Ganji Method, the approximate analytical solutions for the nonlinear equations describing the diffusion-limited reaction in the film are presented in this paper. When compared to the numerical data, the resulting analytical results for the concentrations and current profiles are determined to be in satisfactory agreement. The relationship between the amperometric response and the substrate and mediator concentrations, electrode voltage, enzyme concentration, film thickness, and electrode geometry is also analysed.

4.4 Photo-Electrochemical Water Splitting behaviour of CdSe QDs Sensitized Ferroelectric $SmCoO_3$ Perovskite Heterostructure

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Herein we report the photo-electrochemical water splitting of CdSe quantum dots (QDs) sensitized SmCoO3 perovskite in a sacrificial electrolyte. The CdSe QDs are synthesized via hot injection method and perovskite SmCoO3 is synthesised via hydrothermal synthesis procedure. The CdSe QDs are sensitized to SmCoO3 using mercaptopropionic acid as linker to form heterostructure. The phase purity and crystallinity of CdSe QDs and SmCoO3 are examined using X-ray diffraction analysis and the morphologies are studied using transition electron microscopy (TEM) technique. The optical properties are examined using UV-Vis spectroscopy and the band gap of QDs and perovskite are derived. The XRD analysis of CdSe QDs reveals the high crystallinity with a cubic phase and tetragonal phase for SmCoO3. The surface morphological observations demonstrate that SmCoO3 size in the range of 80-120 nm in size. The TEM analysis reveals single crystalline nature for the SmCoO3 nanoparticles. The optical band gap of SmCoO3 is found to be 3.75 eV and 2.33 eV for CdSe QDs. The CdSe QDs sensitized SmCoO3 heterostructure's photo-electrochemical water splitting behaviour is examined in 1M Na2S electrolyte under 100 mW/cm2 light illumination. As photoanode, CdSe QDs sensitized SmCoO3 heterostructure demonstrated ~39.5 mA/cm2 under illumination and ~32 mA/cm2 in dark at 0.8 V (vs. Ag/AgCl), which implies that photocurrent density of 7 mA/cm2 at 0.8 V (vs. Ag/AgCl). This work discusses the significance and novelty of the usage of CdSe QDs sensitized SmCoO3 heterostructure as photo-electrocatalyst and paves pathway for newer materials development for enhanced photo-electrochemical water splitting.

Key Words: Photo-electrochemical, Water Splitting, Quantum Dots, Perovskite & Heterostructure.

4.5 Extensive investigation ofdelafossite conducting oxides p-type $CuAlO_2$ thin film via chemical solution deposition method

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The transparent p-type copper aluminium oxide (CuAlO2) semiconductor thin film has been synthesized through a cost effective chemical solution deposition method. The effects of post annealing deposition temperature at 450oC for 2 hours with the optimized annealing treatment. The transparent p-type CuAlO2semiconductor thin film was characterized using X-ray diffraction, photoluminescence, FT-IR and XPS analyses. Moreover, all the diffraction line in the XRD pattern clearly exhibits delafossite-type structure and R-3m space group. The photoluminescence studies revealed that the band gap of the CuAlO2 thin film was estimated to be 3.47 eV. In addition, the functional group vibration of the CuAlO2 thin film was confirmed by FT-IR analysis. From XPS analysis, the presence of Cu and Al ions occurs in +1 and +3 oxidations states respectively.

Key words: p-type thin film, delafossite, CuAlO2, Chemical synthesis.

4.6 Comprehensive electrochemical studies on nanolayered multilayered Ti/TiN and TiAl/TiAlN coatings deposited on Ti_6Al_4V substrates

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Corrosion resistance properties of Ti/TiN and TiAl/TiAlN nanolayered multilayered coatings deposited on Ti6Al4V alloy substrates by unbalanced magnetron sputtering were investigated. The coatings contain a bi-layer thickness of Ti/TiN or TiAl/TiAlN

~3.5/4 nm and the total thickness of the coating is ~ 9 µm. Corrosion properties of the coatings were investigated using electrochemical impedance spectroscopy (EIS) for 30 days while immersed in 3.5 wt.% NaCl solution. EIS investigation of the coatings showed that the corrosion occurred due to the penetration of electrolyte and oxygen through the micro/nano pores present in the coatings. It was found that the TiAl/TiAlN coating offered corrosion protection superior to that of the Ti/TiN coating during the immersion study. Potentiodynamic polarization studies revealed that both coatings showed passive behaviour. The formation of a passive film on the coated surface during polarization enhanced the barrier properties of the coatings and provided anodic protection to the underlying alloy.

KEYWORDS: Ti/TiN, TiAl/TiAlN, corrosion properties of Ti/TiN, corrosion properties of TiAl/TiAlN

4.7 An overview on the fabrication of magnetic nanostructures by electro deposition-based methods for advanced applications in molecular electronics.

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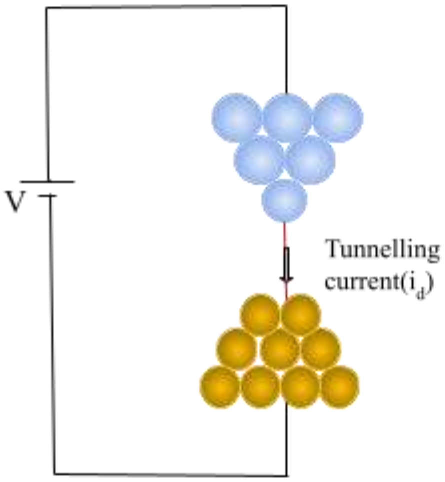
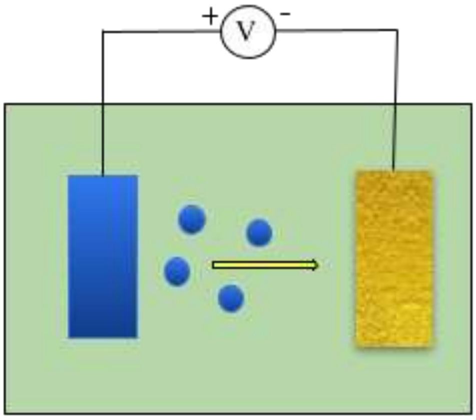
Individual atoms and molecules form the basic entities responsible for most biological and chemical processes. Tuneable nanostructures of such molecules display exceptional macroscopic properties by giving a characteristic and controllable response to a stimulus (like electric/magnetic field, varying temperature and pH). These molecules in ferromagnetic materials show exchange interactions which lead to the molecular ordering of individual spins. Such materials are suitable candidates for spin-selective transport as they are sensitive to magnetic fields, making them promising candidates for applications in quantum computing hardware. The need for molecular electronics is because of the fact that conventional Si-based electronic devices show unpredictable transport behaviour when fabricated at the nanoscale with large leakage current and high power consumption.

Electro deposition is a versatile method for materials protection and metal finishing in various applications such as hard chrome plating. For the fabrication of metallic structures with nanogaps, the distance between two micro fabricated electrodes must be controlled by fixing the tunnelling current with the aid of scanning probe techniques. Increase in the tunnelling current shows a stepwise decrease in the gap between the tip and noble substrate electrodes. This forms an electro deposition like circuit and the atom from the tip is deposited onto the nanometer-scale electrode. It then undergoes structural transformation to attain a stable configuration. Adjusting the electrochemical potential allows us to exploit this behaviour to obtain highly controllable metallic nanostructures. The terminals are held by anchoring groups which hold them by covalent bonds, co-ordinate covalent bonds or through π-π interactions.

Magnetisation is achieved after the accumulation of several atomic layers which is done using electrodeposition on a conductive substrate partially coated by an insulator, forming a nanoscale pattern with conformal growth, exhibiting properties like magneto resistance similar to that of the nanofilms synthesised by vacuum deposition. Porous templates are also used to regulate the nanostructures to ensure no bulk deposition.

Keywords: Molecular electronics, Scanning Probe techniques, Nanomaterial synthesis.





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Micromachines 2022, 13, 1223

Nanomagnetism and Spintronics, pp. 89-120 (2010)

4.8 Electrophoretic Deposition of S53P4 Bioactive Glasses onto Ti alloy

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Bioactive glass (BAG) is a group of bio ceramic that consist silicates and it's structures has ability to form the chemical bond between surface and surrounding tissues especially with bone matrix. Biological response can be enhanced by these classes of biomaterials that can able to form bone like apatite structures and generation of new bone tissues [1]. Electrophoretic deposition (EPD) is a simple, versatile and cost efficient process is being used for deposition of bioactive glass. EPD is two-step process by which the particles suspended in colloidal solution. Particles migration occurs by applied electric field and deposition of charged particles onto working electrode [2]. Biocompatibility, bio mimicking nature of bone matrix and formation of hydroxyapatite facilitates integration of apatite with bone matrix. The colloidal suspensions of S53P4 were prepared and EPD was carried out with optimized parameter including voltage and time. Ti6Al4V substrates were used as working and counter electrode. Distance between working and counter electrode was 3cm. Characterization was done to analyse and confirm the deposition of BAG. FTIR confirmed the presence of BAG onto Ti alloy substrates. XRD were carried out to confirm the amorphous nature of BAG. Morphology of coated substrates were analysed by SEM and elemental composition was observed using EDAX. Surface wettability plays a vital role in cell proliferation or cell differentiation for growth of new tissues. Hydrophilic tendency of BAG would enhance the cell proliferation and promotes better osseointegeration.

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4.9 Facile synthesis of Layered Cobalt Hydroxide ($Co(OH)_2$) Nano-sheets on Copper Electrode for Efficient Electrocatalytic Oxygen Evolution Reaction

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Electrochemical water splitting is an important reaction in catalytic conversion of renewable electrical energy (e.g., solar, wind, geothermal etc.) into hydrogen, which involves a coupled Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER). OER is often considered a hindrance in water splitting because of its sluggish kinetics. The benchmark electrocatalysts, such as IrO2 and RuO2, are less abundant and thus the cost of energy conversion is high. Consequently, there is a significant need to develop catalysts that are cost- effective and have better OER efficacy. Layered transition metal hydroxides are being used for OER, owing to their unique electrochemical properties, high-stability, and high abundance. Herein, we report the galvanostatic electrodeposition of vertically-aligned cobalt hydroxide Co(OH)2 nanosheets on a copper (Cu) electrode. The duration of electrodeposition was optimized based on the electrochemical OER properties. The temporal changes in catalytic activity have been analysed using voltammetry, electrochemical impedance spectroscopy, and electron microscopy techniques. The electrodeposited Co(OH)2 nanosheets shows enhanced electrocatalytic activity with a lower overpotential of 339 mV at 10 mA cm-2 and a Tafel slope of 56 mV dec-1 in alkaline media. These findings provide a compelling fundamental framework for the development of efficient and affordable OER electrocatalyst.

Keywords: Co(OH)2, Oxygen evolution reaction (OER), electrocatalyst, electrodeposition, Copper electrode.

4.10 Electrochemical Investigation on mechanism of As(V) removal from contaminated water

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Water is one of the most important vital necessity of all human Beings. Among the most abundant impurities found in water, arsenic is one of the deadliest toxins. The permissible level of Arsenic in body is 10 µg/L(“Arsenic,” n.d.) as per Indian Water Standard IS 10200:2012. Beyond this level, it serves as a potential threat to the human body. Therefore, arsenic removal from contaminated water for portable purposes is necessary, to reduce its concentration to the mentioned maximum admissible level.

Sacrificial metal based insitu generated adsorbents have served as efficient filter media for As(V) remediation in drinking water. The mechanism primarily involves corrosion of sacrificial metal, formation of oxides and hydroxides and complex formation of arsenite and arsenate with the iron surface and with iron oxides produced from iron corrosion (Rajakovic et al., 2018). This research uses electrochemical methods to investigate the redox reactions that occur on the surface of zerovalent iron in arsenic solutions. The effect of arsenic on the corrosion rate of sacrificial metal was investigated by analysis of Tafel diagrams at different As(V) concentrations. The results indicate that As(V) remediation is heavily dependent on the initial As(V) concentration, type of sacrificial metal, pH and other interfering ions present in water. These factors will provide an insight for the construction of sacrificial metal based arsenic filter for its mitigation in water.

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4.11 Synthesis, Characterization, Electrochemical and DNA binding Analysis of Imidazole based Mixed Ligand Mn^{II}, Co^{II} And Cu^{II} Complexes

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The imidazole-based ligand 2-(4,5-diphenyl-2,5-dihydro-1H-imidazole-2-yl-4-nitrophenyl (im) and their mixed ligand metal complexes (MnII, CoII and CuII) were synthesized and characterized by spectroscopic studies and spectroscopic results were afforded distorted square planar coordination geometry for MnII, CoII and CuII complexes. The DNA binding of these complexes were investigated by absorption spectral titration. The corroborative results of these experiments validate that complexes bind to CT DNA via intercalation binding propensity with binding constant value of 1.42 x 10-3 M-1 for [Cu(im)2], 9.24 x 10-4 M-1 for [Co(im)2] and 1.84 x 10-5M-1 for [Mn(im)2] complex and binding activities of complexes followed the order: [Cu(im)2] > [Co(im)2] > [Mn(im)2]. The electrochemical properties of all the complexes were investigated by cyclic voltammetry and the [CO(im)2 [Co(NO2im)2] complex exhibit one-electron irreversible reduction at -1.5 V, [Mn(im)2] complex exhibit one-electron irreversible reduction at -1.0 V and [Cu(im)2] complex exhibit one-electron irreversible reduction at -1.2 V. This type of DNA binding and electrochemical activity order explained on the basis that the general series found by Irving and Williams for the stability of the complexes.

Keywords: Imidazole based ligand MnII, CoII and CuII, DNA Binding, CT DNA, Electrochemical Properties.

4.12 Pulse Copper Electroplating -Through Hole of Printed Circuit Boards (PCBs)

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Miniaturisation and portability of consumer electronics is driving the ever-increasing circuit density of today's printed circuit board(PCBs) designs. With increasing functionality and complexity of PCBs, industries are demanding for improved properties of deposited copper and uniform deposition of copper.Realisation of such complex technologies adopt complex electroplating process whose outcome depends on numerous factors including the process conditions, type of equipment used and the characteristic of product itself. DC assisted electroplating Copper electroplating is widely used in the PCB industry. Due to inherent technical limitation such as uneven field distribution,"Pulse Electroplating is becoming popular. Today, Pulse plating (PP) equipment is being used in the printed circuit board manufacturing for complex high aspect ratio boards for through-hole copper plating. Thus the plating industry is at the threshold of an entirely new development. Pulse plating is now an accepted technology and is proving to be a very useful tool for the electroplater.The combination of electronics and electrochemistry is proving to be an avenue to open up new ideas and horizons for the electroplating industry. Research and development in that area is therefore not only restricted to enhance the synergistic effect of the various additives, but also to the application of advanced techniques for the metal deposition.In this study, introduction of pulse electroplating technique for through-hole plating of PCBs and effect of pulse parameters on uniformity of plated copper is investigated.

Keywords—Pulse electroplating, DC Electroplating, Plating thickness, pulse parameter Plated-through hole (PTH), Printed Circuit Board , plating distribution, Aspect Ratio.

4.13 Electrocatalytic activity of Co doped RuO_2 towards oxygen evolution reaction in universal pH condition

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The fabrication and development of effective electrocatalyst for water splitting reaction towards the viable H2 production, as an alternative to fossil fuels are inevitable. Moreover, designing of OER electrocatalyst with high stability and activity across the universal-pH condition was highly challengeable. Generally, the structural engineering and electronic modification of the catalyst would synergistically increase the OER performance by increasing the active sites and also the long-term stability in universal-pH. Having this knowledge, herein this work fabrication of Co doped RuO2 via simple wet-chemical method followed by annealing at air atmosphere was employed as OER electrocatalyst in universal pH (=0.3, 7, 8.5 and 14). The catalyst Co-RuO2 exhibits an, overpotential of 238 mV 328, 453, and 470 mV in acidic, neutral, and near-neutral environments respectively, to attain a 10 mA/cm2 current density. Here it is observed that doping of Co into the RuO2 could synergistically increase the active sites with the enhanced electrophilic nature of Ru4+ to accelerate OER in all of the pH ranges.

5. Energy Martials

5.1 Sulfonated poly ether etherketone-basedhybrid proton exchange membranes customized with UiO-66-NH_2 metal-organic frameworks for DMFC applications

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Hybrid proton exchange membranes (PEMs) based on the blends of sulfonated poly (ether ether ketone) (SPEEK) and UiO-66-NH2 were prepared successfully. The fabricated hybrid membranes showed favorable PEM characteristics such as reduced methanol permeability, high selectivity, and improved mechanical integrity. Additionally, these membranes afford comparable proton conductivity, good oxidative stability, moderate ion exchange capacity, and reasonable water uptake. To appraise PEM performance, the blend membranes were characterized using techniques such as Fourier transforms infrared spectroscopy, AC impedance spectroscopy,scanning electron microscopy, atomic force microscopy, and thermogravimetry. Addition of UiO-66-NH2into SPEEK increases the tensile strength of the membrane. The methanol permeability exhibited by the SPEEK/UiO-66-NH2 blend membrane is much lower than that of Nafion-117. The observed results demonstrated that the SPEEK/UiO-66-NH2hybrid PEMsare promising have for possible use in direct methanol fuel cells.

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5.2 Effect of zirconium-based MOF-808 metal-organic frameworks on permeation and antifouling properties of poly (amide imide) ultrafiltration membranes

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In this study antifouling hydrophilic polyamide imide (PAI) ultrafiltration (UF) membranes were successfully fabricated via phase inversion technique using zirconium-based MOF-808 metal-organic frame works (MOFs). The bare PAI and PAI/MOF-808 membranes were characterized in terms of scanning electron microscope (SEM), contact angle (CA), Fourier transform infrared spectroscopy (FT-IR), pure water flux (PWF) and X-ray diffraction (XRD). The FT-IR is employed to probe the surface functionalities on the membranes. The top surface and cross-section scanning electron microscopy (SEM) images evidenced that the incorporated MOF-808 is significantly altered the membrane morphology by causing increased porosity and macrovoid formation on the surface as well as in the bulk of the hybrid PAI membranes. The contact angle (CA), pure water flux (PWF), water uptake and porosity were also measured to evaluate the enhancement in hydrophilicity of PAI/MOF-808 hybrid membranes. The antifouling capacity of the membranes was evaluated using BSA and HA fouling agents. The PAI/MOF-808 hybrid membranes showed an increase in pure water flux, water content and lesser contact angle. The flux recovery ratio (FRR) of the PAI/MOF-808 membranes are increased during the rejection studies of BSA and HA demonstrated their excellent separation and antifouling ability. Overall results evident that the zirconium-based MOF-808 MOFs incorporated PAI UF membranes showed potential for water treatment applications.

5.3 Separation of bovine serum albumin and humic acid using hybrid poly (vinylidiene fluoride) ultrafiltration membranes customized with MOF-801

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Custom-made poly (vinylidiene fluoride) (PVDF) ultrafiltration (UF) membranes with enhanced permeability were synthesized by the addition of zirconium-based metal-organic frameworks (MOFs) MOF-801. The surface roughness and morphology of the as-prepared membranes were studied by atomic force microscopy (AFM) and scanning electron microscopy (SEM) respectively. The wettability of hybrid membranes was measured by water contact angle (WCA) using goniometer. The improvement in pure water flux (PWF) and antifouling ability was noticed after the introduction of MOF-801 into the PVDF membrane matrix. A considerable increase in porosity (38.91%) and roughness whereas decrease in WCA of 55.1o were exhibited by hybrid PVDF membranes at optimal addition of 2 wt.% MOF-801. The rejection and antifouling performance of PVDF and PVDF/MOF-801 hybrid UF membranes were tested by protein (BSA) and natural organic matter (HA). The FRR was found to be increased from 66.4 to 89.6% and 68.3 to 85.2% for BSA and HA separation indicates the enhanced antifouling property of the PVDF hybrid membranes. Besides, from the zone of inhibition test the antibacterial ability of hybrid PVDF UF membranes against E. coli and S. aureus was found to be greatly improved by the addition of MOF-801. Overall results demonstrated that the PVDF/MOF-801 hybrid membranes are potential for treating the waste water.

5.4 Synthesis of Spinel Copper Cobaltite/Copper oxide nanocomposite for Energy and Environmental Applications

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Spinel Metal Oxide nanomaterials have been extensively studied for various energy and environmental applications including energy storage, energy conversion and environmental remediation. Spinel (AB2O4) structured materials have unique properties subsequently used in numerous fields such as magnetic, optics, electricity and catalysis. Spinel Oxide materials are environmentally friendly and cost-effective, which makes them as a promising material for Energy and Environmental Applications. In this work Cu0.15Co2.84O4-CuO nanocomposites were synthesized by different methods such as Hydrothermal, Microwave and Precipitation. The prepared nanocomposite material has been characterized using X-ray diffraction pattern, Raman spectra, Scanning Electron Microscopy, Transmission Electron Microscopy and X-ray Photoelectron Spectroscopy. The photocatalytic behavior of Cu0.15Co2.84O4-CuO nanocomposite was studied by using degradation of methylene blue dye under UV light irradiation. I-V characterization was studied for evaluate the photovoltaic performance of Cu0.15Co2.84O4-CuO nanocomposite based devices. The results showed that the synthesized nanocomposites have excellent photovoltaic and photocatalytic behavior.

Keywords: Cu0.15Co2.84O4-CuO nanocomposites, photovoltaic performance, photocatalytic degradation.

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5.5 Ion-conducting behavior of electrospun nano-composite quasi-solid electrolyte for an efficient performance of Dye-sensitized solar cells

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The ion-conducting behavior, relaxation dynamics and the photovoltaic performance of the nano-composite electro-spun PVDF-HFP/ x wt% of nanofibrous TiO2 (x = 2, 4, 6, 8 wt%) electrolyte membranes were studied. As the reported electrolyte membranes are highly ion-conducting, random barrier model was used to interpret the conduction mechanism and found the dominance in electrode polarization effect. Moreover, the relaxation dynamics were analyzed by Havarliak- Negami formulation. Among the prepared nano-composite polymeric electrolytes, PVDF-HFP/ 6wt% nanofibrous TiO2 membranes with Li based electrolyte shows high conductivity and exhibited a high PCE of 7.02% for the fabricated DSSC. The photovoltaic parameters of the fabricated DSSCs were extracted using an equivalent circuit of single diode model of generalized solar cells to interpret their influence in the photovoltaic performance.

Keywords: Electrospinning, PVDF-HFP/ x wt% of nanofibrous TiO2 TiO2, Random barrier model, Havarliak- Negami formulation, Dynamic relaxation.

5.6 nvestigation of Copper Oxide Hole Transport Layer in Planar Perovskite Solar Cells

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Copper Oxide nanoparticles (CuO NPs) have been widely studied as a hole transport material in photovoltaics and optoelectronic devices owing to their suitable band gap, high hole mobility, good conductivity, good chemical stability and low cost. In this work, precipitation (P-CuO), microwave (M-CuO) and hydrothermal (H-CuO) assisted methods are used to prepare the copper oxide nanoparticles. The physical and chemical properties of CuO NPs are characterized by X-ray Diffraction (XRD), Raman spectroscopy, X-Ray Photon Spectroscopy (XPS), Scanning Electron Microscopy (SEM) Transmission Electron Microscopy (TEM) and UV-DRS Spectroscopy. The prepared CuO NPs were employed as a hole transport materials in the planar perovskite solar cells. H-CuO-based devices achieved a maximum power conversion efficiency of 7.75% with a photocurrent of 16.98 mA/cm2 and retained the stability for more than 1000 hours. The power conversion efficiency of P-CuO, M-CuO- based device is 3.46%, 5.43%, respectively. The hydrothermally prepared CuO (H-CuO) based device exhibits the highest power conversion efficiency (PCE) compared to other devices. Impedance analyses provide evidence of good interfacial contact, enhanced charge extraction/transport and suppression of charge recombination. Meanwhile, the H-CuO-based device shows better device stability compared to the without-HTM and P3HT-based devices.

Key words: Perovskite Solar Cell, Copper Oxide, Hole Transport Material.

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5.7 Surface modification of MnV- Layered Double Hydroxide nanosheets coupled with MXene electrode for Flexible Hybrid Supercapacitor

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Layered double hydroxides (LDHs) of transition metals have attained significant attention for supercapacitor applications due to their excellent charge storage, low internal resistance, and superior electrochemical stability. However, the restacking of LDHs and poor conductivity still limit their further application. To address these critical issues, in this work, the MnV-LDH/MXenes nanosheet composites with strong contact have been fabricated by introducing MXenes as the structure-directing substrate. It is found that MnV-LDH can duplicate the MXene structure to generate sufficient contact, accelerating the electron transfer and exposing abundant electroactive sites to enhance the electrochemical kinetics. Because of these advantages, the as-made MnV-LDH/ MXenes electrode shows a good specific capacitance of 1853 F g–1 at 1 A g–1 with capacitance retention 86% retention of capacitance after 10,000 cycles. This planar supercapacitor device is a new strategy to fabricate the stretchable micro-supercapacitor devices for wearable electronic applications.

Keywords: Surface Modification, MnV- LDH, Mxene, High Energy density, Flexible Device

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5.8 N, B Dual Heteroatoms Doped Porous Carbon for Symmetric Supercapacitor application

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The N and B dual heteroatom doped carbon is an excellent candidate for enhancing the supercapacitor performance owing to its high surface area, and active sites. In this work, we have developed a rod like nitrogen and boron dual doped porous carbon (NBPC) with the aid of the SBA-15 as a supported material and examined the doping effect toward supercapacitor performance. The resulting NBPC material establishes a high surface area (809 m2/g), a large pore volume (0.16 cm3/g) and higher amount N and B species, which offers remarkable supercapacitor activity. In addition, NBPC showed a high specific capacitance (375 F/g) at 2 A/g current density in 1 M H2SO4 electrolyte with higher rate capability and capacitance retention. Moreover, the introduction of dual redox additive materials to the electrolyte, enhanced the specific capacity of the fabricated symmetric supercapacitor cell providing a high specific capacity of 929 C/g at 3 A/g current density, and 56% of the initial specific capacity was retained when current density increased to 20 A/g. The fabricated cell delivered a high specific energy and power density of 48.4 Wh/kg and 15 kW/kg which are five folds higher than the bare electrolyte's (10.1 Wh/kg and 5 kW/kg), respectively.

5.9 Synthesis and Characterization of Iron Oxide Nanoparticles for Supercapacitor Application

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Iron oxide nanoparticles were prepared in various concentrations at constant temperature by hydrothermal method. From the results of UV-VIS it is revealed that the absorption wavelength is at 320nm and the band gap value is 1.67eV which is calculated using Kubelka Munk method. Photoluminescence spectrum revealed the excitation wavelength at 360nm and emission wavelength at 680nm due to red emission. Iron oxide nanoparticles are used for supercapacitor application on account of its band gap value.

Keywords:UV-VIS, PL and Supercapacitor.

5.10 Cerium and molybdenum selenide-based composites as efficient electrodes with prominent cyclic stability for supercapacitors applications

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Cerium and molybdenum-based chalcogenides were used extensively as electrode materials in energy storage applications due to their multiple oxidations state, good electrocatalytic ability, and electrochemical properties. Herein, Cerium selenide and molybdenum selenide composites (CeSe/CeSe2/MoSe2) (CEMSE) were synthesized by a single-step hydrothermal method by varying cerium and molybdenum metal ratios (Ce:Mo) represented as CEMSE 1:1, CEMSE 1:2 and CEMSE 2:1. The structural and morphological studies were analyzed using XRD and SEM, respectively. The elemental composition, chemical, and electronic states of the prepared composites were analyzed by XPS analysis. The charge storage ability of the composites was tested under various electrochemical techniques such as cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). Compared with single metal chalcogenides and other metal ratios composites, the CEMSE 1:1 composite showed a high specific capacitance of 260.50 F g-1 at the specific current of 1 A g-1 obtained from the three-electrode system. The symmetric supercapacitor was fabricated with CEMSE 1:1 material, and it showed specific energy of 7.7 Wh kg-1 with a specific

power of 599.89 W kg-1 at a specific current of 1 A g-1. The symmetric device withstands up to 5,000 cycles and shows high columbic efficiency of 100 % with capacitance retention of 80 %.

Keywords: Chalcogenides, Hydrothermal method, Cyclic voltammetry, Galvanostatic Charge-Discharge study, Electrochemical Impedance Spectroscopy, Specific capacitance, Columbic efficiency, Capacitance retention.

5.11 Electrochemical preparation and investigation of Polypyrrole- carbon quantum dot - copper electrode for supercapacitor applications

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Supercapacitor (SC) is an energy storage device that can store electrical energy by an ion or electron transfer mechanism. Carbon sources, metal oxides, and conducting polymers are used as electrode materials for SC applications. Among these, polypyrrole (PPy) is a conducting polymer that has much more attention due to reversible redox behavior and high capacitance behavior. However, it suffers from low electrochemical stability because the polymer chain easily brokes when it involves a long-term charge and discharge process. To overcome this issue, additive materials like carbon, nitrides, sulfides, and metal oxides are doping to the polymer chain. In this work, we prepare carbon quantum dot (CQD) is low-cost and highly efficient carbon material and doped the pyrrole chain by electropolymerization. In addition, boosting the capacitance behavior the copper (Cu) metal is added to the PPy-CQD composite. The prepared PPy-CQD-Cu electrode material's electrochemical behavior was characterized by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and galvanostatic charge-discharge techniques. The electrode exhibits 244 F/g specific capacitance at 1A/g current density is higher than the undoped PPy electrode. Then, we fabricate the two-electrode system in which activated carbon (AC) is a negative electrode and PPy-CQD-Cu is a positive electrode. The device delivered 30.60 wh/kg energy density and 902.95 w/kg power density and gave 88% capacitance retention after 3000 cycles. The above

result suggests that the PPy-CQD-Cu is an efficient electrode material for supercapacitor application.

Key words: Polypyrrole, Electropolymerization, Carbon quantum dot, Supercapacitor.

5.12 Chronoamperometric deposited W40Se (2.5, 5, 10) on L-Cysteine doped Artocarpus Heterophyllus peel derived carbon wrapped on Ni-foam for enhanced Hybrid Supercapacitor Applications

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In this study, we have electrodeposited W40Sex (X= 2.5, 5 & 10 mM) in a chronoamperometric technique upon switching the potential with customized relaxation time, decorated NSC3 on Ni-foam and studied their effective supercapacitor applications. The diffraction pattern obtained concerning JCPDS card no: 06-0080 confirms crystallinity and formation of hexagonal WSe2 through the XRD technique. The chemical bonding and functional group of synthesized CWSe0.25, CWSe5, CWSe10 composite and bare NSC3 are confirmed by FT-IR spectroscopy. Notable, decrease in the -OH, -C-S, -C-S-C peak intensity with an increase in Se-concentration highly suggests the formation of thick WSe2 layers. The structural properties were analyzed with the RAMAN spectrum to confirm the availability of Se-Se vibration. The good reversibility and enhanced capacitance behavior of the composite electrode is being revealed by cyclic voltammetry results. Moreover, EIS results demonstrate that the composite of CWSe5 has better ionic conductivity than CWSe0.25, CWSe10 and bare NSC3. The composite of CWSe5 has a capacitance of 825 F/g which is higher than the bare NSC3 305 F/g at 1 A/g. After 1000 cycles, CWSe5 composite electrode exhibited enhanced capacity retention of 75% and the bare NSC3 was 33%.

Keywords: Electrodeposition; chronoamperometric; NSC3; WSe2; L-cysteine.

5.13 Electrochemical Investigation of High-Performance Supercapacitor based on Novel 2D Ru-Nb_2O_5@Sbnene Nanosheets

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Two-dimensional (2D) materials with superior electrochemical properties have been intensively investigated for the fabrication of high-performance supercapacitor electrodes for future energy storage applications. In this present work, we have successfully synthesized Sbnene-nanosheets and embedded Ru-Nb2O5 nanoparticles into the interstitial position of the nanosheets for high-performance supercapacitor application for the first time. The synthesized nanosheets were characterized XRD, SEM and FT-IR spectroscopy. The availability of Nb2O5 improves supercapacitor conductivity, which can aid to increase the overall efficiency and performance of the as-fabricated Ru-Nb2O5@Sbnene nanosheets. Also, the incorporation of Ru-Nb2O5 into Sbnene-nanosheets specifically lowered the restacking of the nanosheets functioning as spacers in between the layers of Sbnene-nanosheets. As a result, the electrochemical results retrieved from the three-electrode set-up reveal that the composite nanosheets demonstrate a high integral area with a specific capacitance of 450 F/g at 10mV/s. The electrochemical impedance spectra (EIS) showcased low solution resistance and charge transfer resistance of 0.2 and 2.4 Ω respectively. Besides, the Ru-Nb2O5@Sbnene nanosheets possess long charge-discharge and high-rate capabilities owing to the addition of Ru-atoms in Sbnene-nanosheets provides more electroactive sites, which improves overall electrochemical performance and charge storage capacity.

Keywords: Two dimensional materials; ruthenium; niobium oxide; Sbnene-nanosheets; supercapacitors.

5.14 Synthesis and characterization of Torlon- SPEEK-sulfonated silica proton conducting polymer electrolytes for PEM fuel cell applications.

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Fuel cells have received much attention for clean power generation for transportation, portable power systems, etc. In the present work is sulfonated poly (ether ether ketone) / poly (amide imide) Torlon were prepared for various conditions such as percentage compositions of the SPEEK blend with sulfonated silica. The NMR, IEC analyses confirmed the degree of sulfonation level as 65%. The prepared composite membranes were characterized by using Fourier transform IR spectroscopy. Surface morphology of the acid-base composite membranes was analyzed using scanning electron microscopy and atomic force microscopy. Other physical properties related to conductivities ion exchange capacity, proton conductivity and durability were also evaluated for the prepared composite membranes. The water uptake, swelling ratio and Lambda value of prepared films were studied and the proton conductivities at were measured. These composite membrane showed good proton conductivities and durability and expected to be used in the development of H2/O2 fuel cells.

Key words: SPEEK, PAI, NMR, SEM, acid-base composite.

5.15 Recent advances in the improved electrochemical performances of cathode materials for Li-ion battery

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SiO2 coated LiNi1/3Mn1/3Co1/3O2 particles prepared by sol-gel method. The structure and electrochemical properties of the surface modified LiNi1/3Mn1/3Co1/3O2 materials were characterized by systematically investigated using XRD, SEM, Cyclic voltammetry and Charge-discharge techniques. The cycling behaviors of SiO2 -coated LiNi1/3Mn1/3Co1/3O2 cathodes were evaluated with various discharge rates between

4.2 and 2.9V. The initial discharge capacities of 192, 217, 237, 267mAh/g respectively, and maintain the excellent cycling behavior with little capacity loss. It is very clear from the result that, the irreversible capacity for the first cycle is very minimum for 3 wt % SiO2 – coated LiNi1/3Mn1/3Co1/3O2 compared with uncoated and other coated electrode. 3wt % silica coated LiNi1/3Mn1/3Co1/3O2 had the highest Initial charge and discharge capacities than pristine compound and other silica coated samples. These coated samples suggest The initial discharge capacity for cathode that even for the coated layered phase more amount of Ni2+, Mn4+and Co3+ has contributed to the charge and discharge capacities during electrochemical reactions. This cycling behavior of the SiO2-coated LiNi1/3Mn1/3Co1/3O2electrodes indicates the impact of SiO2coating considerably which improved the electrochemical performances. On the other hand, 3.0 Wt.% of SiO2-coated LiNi1/3Mn1/3Co1/3O2 shows the similar characteristics of two potential plateaus which were obtained at 2.9 and 4.2 V compared with the uncoated electrode. Electrochemical tests SiO2 incorporation (3 wt %) can significantly improve the electrochemical performance, especially at high C-rates, enhanced structural stability.

Key words: Cathode materials, Li - ion battery, Sol-gel, Coating material.

5.16 Electrochemical performance and investigations of Ferric Oxide/ β-cyclodextrin composite material for supercapacitor

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The development of an efficient synthesis process for carbon-based supercapacitor electrodes is highly appreciated for its practical application. Iron oxides have been widely recognized in the energy storage field, owing to their high theoretical capacitance, low cost, and environmental friendliness. However, the intrinsic poor electrical conductivities have significantly hindered their practical applications. The rational design of the conductive supports is considered an efficient approach to solving the issues. In this work, Fe2O3 was encapsulated in carbonized β-cyclodextrin (β-CD) by

hydrothermal method and analyzed electrochemical behavior in the negative potential window. The Fe-β-CD composite gives a high specific capacitance of 340 F/g at 1 A/g and excellent cycle durability with 100% capacitance retention after 1000 cycles at 5 A/g. Then, the cobalt is doped with the resultant Fe-β-CD composite. The Fe-Co-β-CD composite electrochemical behavior was analyzed in the positive potential window which delivers a high specific capacitance of 155 F/g at 1 A/g and excellent cycle durability with 87.5% capacitance retention after 1000 cycles at 5 A/g. The superior electrochemical properties of Fe-β-CD and Fe-Co-β-CD are favorable for ion storage and electron transfer property due to the synergistic effects of high specific surface area and well-balanced micro/meso porosity. Moreover, a quasi-solid-state hybrid supercapacitor is assembled using Fe-β-CD as an anode and Fe-Co-β-CD as the cathode. The above result suggests that the Fe- β-CD // Fe-Co-β-CD asymmetric device is a promising candidate for practical supercapacitor application.

Keywords: Iron oxide, β-cyclodextrin, synergistic effect, asymmetric supercapacitor,

5.17 MXene/Carbon Composite for Highly Efficient Long Life Supercapacitor

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Supercapacitors (SCs) are considered as potentially modicum solution for short-term energy storage because of their high power density and long cycling life. They are capable of charging and discharging electrical energy quickly. MXenes, which are transition metal carbides, nitrides, carbonitrides with layered morphology, mechanical stability and large electronic conductivity has gained intensive research attention in the recent years. The restacking issue of this promising electrode material has been circumvented with spacers like CNT, graphene, polypyrrole, etc., An in-situ etched and subsequently heat-treated Titanium carbide/carbon heterostructure by high temperature treatment, where carbon decorated MXene is synthesised for ultrahigh conductivity and capacitance. This composite electrode material delivered an excellent

specific capacitance of 510 F/g by virtue of its excellent charge storing capability. Also, the composite electrodes with symmetrical aqueous arrangement delivered an outstanding energy density and power density with excellent stability. The prepared nanocomposite electrode exhibiting a synergistic effect of enhanced conductivity and structural stability can be used to explore the commercial viability. The preparation and characterization of MXene/carbon composite and its electrochemical performance in supercapacitors will be discussed in detail.

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5.18 $LaFeO_3$ as a bi-functional oxygen electrocatalyst for electrically rechargeable Zinc-air batteries

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The zinc-air battery is a promising battery system due to its high theoretical energy density and low cost1. The theoretical energy density of a Zinc-air battery is 1086 Wh kg-1, which is five times greater than that of lithium-ion batteries1. Furthermore, zinc metal is one of the most abundant metals in the earth's crust and is relatively cheap. Rechargeable metal-air batteries work on the principle of two fundamental electrochemical reactions known as the Oxygen Reduction Reaction (ORR) during discharge and the Oxygen Evolution Reaction (OER) during recharge2. The performance of the battery will be determined by the bifunctional electrocatalyst's electrocatalytic activity towards two oxygen reactions3. Recent advancements in catalyst development are the fabrication of rechargeable air electrodes using a single active material that is capable of bifunctionally catalyzing ORR and OER3. The development of high-activity bifunctional catalysts is required for rechargeable metal-air batteries such as zinc-air batteries2.

In this work, a perovskite-type LaFeO3 material was synthesized using a citric acid-assisted sol-gel method and is investigated as a bifunctional oxygen electrocatalyst for electrically rechargeable zinc-air batteries. X-ray diffraction structural studies demonstrated the formation of phase pure LaFeO3 in space group Pbnm. This catalyst displayed considerable bifunctional catalytic activity for both oxygen reduction (0.74 V vs. RHE) and oxygen evolution reactions (0.40 V vs. RHE at 10 mA cm-2) in 1 M KOH electrolyte. After the first discharge, electrically rechargeable zinc-air batteries constructed with LaFeO3 as the oxygen electrocatalyst have a specific capacity of 1102 mAh g(Zn)-1. Further details will be provided during the oral presentation.

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5.19 Supercapacitor performance of hydrothermally prepared transition metal diselenides (TMS, M = V, Mo, Co, Ni): A comparative study

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We compared the supercapacitor performance of different hydrothermally prepared transition metal diselenides (TMS, where M = V, Mo, Co, and Ni) nanostructures. TMS supercapacitor electrodes were fabricated by using the drop-cast method on the Ni-foam (NF) [1]. The comparative supercapacitor performances were studied by cyclic voltammetry (CV), galvanostatic charge and discharge (GCD), and electrochemical impedance spectroscopy (EIS) in 3M KOH solution as electrolyte. From the GCD results, the specific capacitance of CoSe2, NiSe2, VSe2, and MoSe2 was measured to be 584.2, 325.5, 133.1, and 81.3 F/g, respectively. As a result, CoSe2 shows better performance than NiSe2, VSe2, and MoSe2 because of its electrochemically large active surface area, which contributes to efficient charge transport and high electrical conductivity [2]. The order of supercapacitor performance is CoSe2 > NiSe2 > VSe2 > MoSe2. Thus, the current study on the comparative energy storage performance of TMS shows that CoSe2 might be further explored as a viable material for energy storage applications.

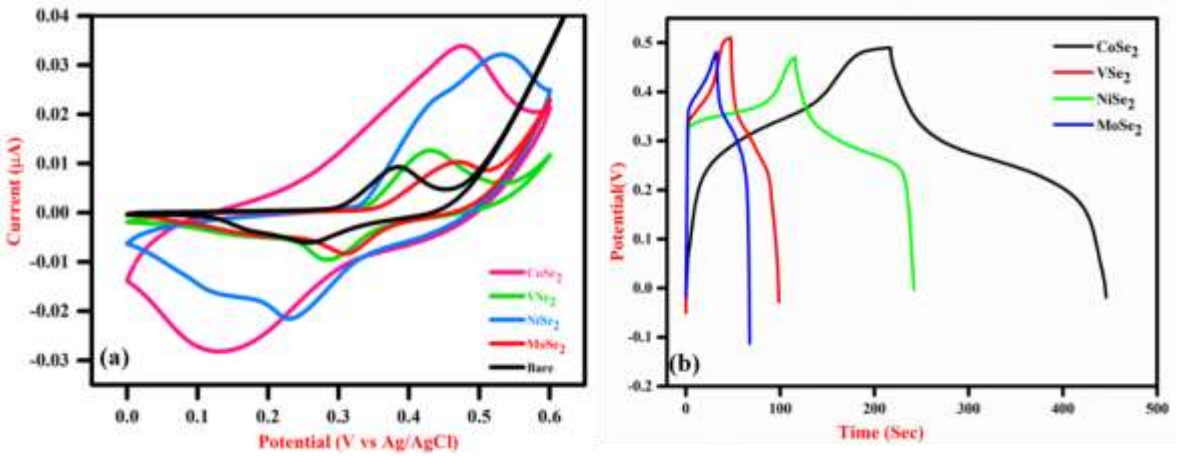

Figure: (a) Comparison of CV responses of bare NF, and TMS (M = V, Mo, Co, and Ni) at a scan rate of 50 mV/s and (b) Comparison of GCD curves of TMS (M = V, Mo, Co, and Ni) at 1.25 A/g.

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5.20 Porous 0D-Carbon nanospheres derived from Lignocellulose of Artocarpus heterophyllus peel precursor for supercapacitor performance

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Carbon nanospheres (CNS), a zero-dimensional (0D) substance, have emerged as a viable material in energy storage devices, however, cost-effectively generating CNS from raw biomass remains a significant hurdle. Besides, these hemicelluloses are particularly interesting biomass resources for carbon nanosphere (CNS) preparation. Herein, we used hydrothermal carbonization followed by pyrolysis activation method to convert the cellulose enriched biomass of Artocarpus heterophyllus (AH) peel waste into 0D-carbon spheres for the first time. The peel waste of Artocarpus heterophyllus comprises of 50-70% of lignocellulose and 15-30% of hemicellulose and lignin with total composition of 20-30%. The 0D structures of the AH-based CNS have strong electrical conductivity and huge specific surface areas. When used as an electrode material for supercapacitors, CNS demonstrated greater specific capacitance, rate capability, and cycle stability than standard carbon spheres, active carbon, and reduced graphene oxide. According to the rectangular plateaus of cyclic voltammograms, the specific capacitance is 680.6 F g-1 at a scan rate of 20 mVs-1. Additionally, the probable process of CNS synthesis from lignocellulose and hemicellulose was addressed. This work not only demonstrated the EDLC behaviour of the produced 0D-CNS, but it also offered a novel technique for synthesizing high capacitance and stable biomass-based electrode materials.

Keywords: Zero dimension; carbon nanosphere; Artocarpus heterophyllus; biomass; supercapacitors

5.21 Preparation of cobalt oxide doped carbon quantum dot (CQD) nanocomposite and evaluate their electrochemical performance for supercapacitor application

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Carbon materials like graphene, carbon nanotubes, and quantum dot doped metal oxides have much more attraction in energy storage applications owing to their sufficient surface area and efficient electrochemical activity. In this present work, carbon quantum dot (CQD) doped cobalt oxide (Co2O3) composite (Co-CQD) was prepared using cobalt nitrate and ascorbic acid (carbon source) through a facile hydrothermal method. The composite material functional groups, composition, and surface morphology were evaluated by XRD, Raman, XPS, SEM, and TEM analysis. The electrochemical performance was studied using a three-electrode setup, the Co-CQD delivers 1209 F g-1 at 1 A g-1 and the capacitance value remained stable after 3000 charge-discharge cycles. The asymmetric supercapacitor was constructed by activated carbon (AC) and Co-CQD (Co-CQD//AC) as the negative and positive electrodes, respectively, which provide 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-CQD is a suitable electrode material for commercial supercapacitor applications.

Keywords: Ascorbic acid, Carbon quantum dot, Hydrothermal method, Supercapacitor.

5.22 Synthesis of $MnNi_2O_4$/ PPy Composite as an Alternate Electrode Material for Future Generation Supercapacitors

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The modern world needs energy storage technology that is both cost-effective and efficient. Due to the significant characteristics of supercapacitors, they are used in energy storage and conversion systems. When compared to batteries, however, they have low energy density. As a result, numerous researchers are continuously addressing the shortcomings in this domain. In the current work, MnNi2O4/PPy, a nanostructured and electrochemically active composite was synthesised. In addition, different physio chemical characterization techniques such as FT-IR, XRD, FE-SEM, EDX and XPS analysis as well as cyclic voltammetry studies were performed. Finally, the composite material,

MnNi2O4/PPy was identified as one of the Potential candidates for energy storage devices.

Key words: low cost, Supercapacitor, Cyclic Voltammetry.

5.23 Hydrothermal Synthesis of Bimetal Oxide/g-C_3N_4 Based Nanocomposites For Enhanced Supercapacitor Applications

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One of the most serious problems confronting mankind today is the depletion of non-renewable fossil fuels such as oil and coal due to large consumption of them for energy. The escalating energy crisis has accelerated the development of new energy sources and energy storage devices. Electrochemical supercapacitors are a promising class of electrical energy storage devices due to their many advantages, including high power density, fast charge- discharge capability, good cyclic stability and excellent reversibility. Cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic charge-discharge lifespan are used to investigate the electrochemical performance of the as-prepared samples. A simple hydrothermal method was used to synthesis CuBi2O4 microspheres. The crystallinity, morphology, chemical composition, and spectroscopic properties of CuBi2O4 studied using FT-IR, XRD, Raman, SEM etc., The electrochemical properties of the proposed electrode were examined using cyclic voltammetry and galvanostatic charge-discharge using 3M KOH electrolytes. The results showed an excellent long-term cycling stability (80% capacitance remained after 500 charge-discharge cycles) and a maximum specific capacitance of 647 F g -1 at a current density of 1.0 A g -1 in 3M KOH. Hence the present material can be a promising electrode material for energy storage devices.

Key words: CuBi2O4 microspheres; Hydrothermal method; electrode material; supercapacitor

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5.24 Effect of surfactant on structural, surface morphology, optical and electrical properties of CuO-NiO/n-Si thin film and its P-N diode applications by drop casting method.

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In this proposed wok, the composite of CuO-NiO thin film were deposited by drop-casting method on commercially purchased n-type silicon wafer substrate which is investigated P-N diode application. The influence of non-ionic surfactant Triton X-100 added CuO-NiO composite which is significant impact on structural, optical and diode properties. From the X-ray diffraction analysis, the films were polycrystalline with an monoclinic and cubic structure of CuO, NiO respectively. The FE-SEM images displayed identical particle for CuO and NiO consequently, bulk flakes deposited for CuO-NiO composite. The elements of Cu, Ni and O presence were confirmed by the energy dispersive X-ray spectroscopy analysis. TEM analysis is confirmed that, the influence of Triton X-100 which is reduced the particle size of CuO-NiO. From the UV-visible analysis, the Triton X-100 modified the bandgap (Eg) value for due to the broad absorbance spectrum. The photoluminescence (PL) behavior of electron-hole pair was investigated. Current-voltage (I–V), characteristics, photo-diode parameters of the Triton X-100 added CuO/NiO/n-Si diode were evaluated under dark and light exposed conditions. To calculate the diode parameter values of ideality factor (n), barrier height (Ub) and sheet resistance (Rs), we have used different methods of I–V, Cheung's and Norde. Photodiode parameters and I–V analysis revealed that Triton X-100 is appropriate for the development of high-quality photodiode and photo detector applications based to its electrical performance.

Keywords: Thin films, XRD, TEM, Thin films, P-N diode, Drop-casting.

5.25 Effect of 2D Tungsten Diselenide Coating on NAM/LNMO Cathode Materials For L-Ion Battery

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Lithium-ion batteries (LIBs) have enormous potential for devices and electric vehicles applications. All the cathodes used for high-capacity/high-voltage have excrusted. A big problem of capacity fading and increasing charge/discharge voltage hysteresis during cycling, stability limitations that hinder real-time applications. Accordingly, several approaches including doping, surface coating, applying active electrolyte additives, and modifying conventional separators have been found beneficial for improving the physicochemical properties of electrodes in rechargeable lithium batteries. Surface coating is the best approach to modify the lithiated transition-metal oxide cathodes in Li/Li-ion batteries and improve their electrochemical behaviour in terms of stability and rate capability. Here, functional surface coatings were applied on (LNMO) and Ni-rich (NAM) NAM cathode materials using few-layered 2H tungsten diselenide (WSe2). Simple liquid-phase mixing with WSe2 in IPA and low-temperature (130 °C) heat treatment in nitrogen flow dramatically improved electrochemical performance, including stable cycling, high-rate performance. A modified and stable SEI was apparently formed owing to W and Se deposition on the Li anode during cycling. The synergistic functionalization provided a significant dual benefit of cathodic and anodic stability.

Keywords: li-ion battery, Tungsten diselenide, Transition metal oxide, Surface coatings

6. Environmental Chemistry

6.1 Integrated Waste Management: [Environmental Science]

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Considering the state of the world today, integrated waste management is crucial everywhere. If the process is not carried out correctly, it results in the worst environmental conditions and has an impact on people's health. In this instance, hospital waste management and hospital equipment sterilization are crucial to the medical sector. Based on the principle that sterilising equipment with ethylene trioxide sterilization or hydrogen peroxide sterilization causes the release of a harmful gas compound called ethylene chlorohydrin. The toxic fumes released by the sterilizer machines used in large-scale hospitals pollute the environment and cause cancer in people.

The gas that the sterilizer machine emits is quite dangerous. We have developed a technique to reduce detrimental to the environment based on integrated waste management because, in general, poisonous gases are difficult to filter. Therefore, when gases enter the machine's vent, the cooling water system treats them, and the polluted water is then treated further to reduce their toxicity.

6.2 Physico Chemical Analysis of Bore Well Water near Solid Waste Dump Site in Thiruvarur District, Tamilnadu, India

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Ground Water samples were collected from ten bore wells located near the Municipal Solid Waste (MSW) of Thiruvarur, Tamilnadu State, India. The samples were collected and sent to the laboratory within six hours for analysis. The physico chemical parameters like Total Solid (TS), Total Dissolved State (TDS), pH, Electrical Conductivity (EC), Total Alkalinity, Chloride,

Biological Oxygen Demand (BOD), and Hardness were studied. During the study, it was determined that TDS ranges from 931 mg/l to 272 mg/l, Chloride ranges from 390 mg/l to 124mg/l and Total Hardness value from634 to 196mg/l. From the observation, it was concluded that some of the results exceed the permissible level of World Health Organization (WHO). Therefore the soil parameters in study area have influenced leachate migration.

Keywords: Municipal Solid Waste, TS, TDS, EC, BOD, WHO, Leachate

6.3 Sustainable approach to Reutilize the Denim Waste using Nitric Acid

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Clothing is considered an important basic need of human life. Nowadays clothing consumption increases because of fast fashion culture among consumers. Because of customers' careless behaviour (take, use, throw away), increases the clothing waste generation. Several million tonnes of textile waste are produced annually around the world, and are anticipated to grow dramatically. Only a very few percentage of waste is reused or recycled back for clothing purposes, however, remaining waste is either dumped as landfills or incinerated. Particularly in the denim industry, a large amount of post-consumer denim waste has been generated every year. The waste produced in textile industry poses serious threats to the global ecological conditions. Thus there is an urge for sustainable options like reducing(minimizing), reusing or recycling denim clothing waste.

The objective of this research is to devise a sustainable approach to reutilize the denim waste by stripping the colour using nitric acid. Colour stripping is the process of removing the colouring component i.e. dyes from the denim material to create a colour free recycled material which may be printed or dyed again with different colours or embroidery can be added for value addition. Box and Behnken statistical experimental plan was used to prepare samples based on the design (15 samples). The effect of Nitric acid on decolourizing the denim garment by varying the processing parameters like concentration of nitric acid (10%, 20%, 30%), Time (5min, 10min, 15min) and Temperature (35℃, 45℃, 55℃) has been

studied and also investigated using response surface methodology tool. It was found that nitric acid can successfully remove the indigo dyes on denim without affecting much of the denim fabric tensile properties. Sample D6 showed better results in terms of tensile strength and colour strength(K/S). Also, the nitric acid used for colour stripping process has been regenerated using activated carbon.

The regenerated nitric acid is used again for the colour stripping process and checked for its efficiency. This regeneration technique is used for three cycles and it was observed that 96% recovery rate has been achieved at every regenerating cycle of used nitric acid. Additionally, the colour stripped denim material was bleached using Hydrogen peroxide and dyed using cold brand reactive dyes. Colour stripped denim garment has been subjected to various tests like tensile strength, whiteness index, Colour strength(k/S) and csharacterized using Fourier Transform Infrared Analysis, SEM and Optical Microscope analysis. Thus a sustainable approach to reutilize the denim waste was studied and critically analysed.

6.4 Conducting Polymer-Based Microbial Fuel Cell for Wastewater Treatment

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Microbial electrochemical systems are a fast-emerging technology that uses microorganisms to harvest the chemical energy from bioorganic materials to produce electrical power. Due to their flexibility and the wide variety of materials that can be used as a source, these devices show promise for applications in many fields including energy, environment and sense. Microorganisms that can produce an electrical current in microbial fuel cells have risen in recent years. Because they do not require the usage of metal catalysts at the anode, microbial fuel cells (MFCs) are exceptional in this regard. Instead, they use microbes that biologically oxidise organic material and send electrons to the anode. Through a circuit, these electrons move to the cathode, where they join forces with protons and a chemical catholyte, such as oxygen. This whole process is carried out in the electrochemical method. Cow dung contains a variety of microorganisms, including endospore-forming Bacillus spp, Enterococcus, and protozoa, which are treated aerobically and anaerobically while

continually supplying the system with the nutrition glucose and urea in phosphate buffer saline (PBS) solution at a pH of ~7. In a doped bacteria chamber, the bacteria are deposited on polyaniline-coated graphene electrode. To establish energy balance, the electrode was tested in both the production of electricity and the treatment of wastewater. MFC eco-friendly and green technology cleans the wastewater using bacteria and the organic matter oxidised to produce electricity.

Keywords: Microbial Fuel Cell, Phosphate Buffer Saline, Bacillus spp, Cow Dung, Polyaniline coated graphene sheet electrode, Wastewater treatment.

6.5 Statistical Analysis to Evaluate the Photocatalytic Activity of Titanium Dioxide

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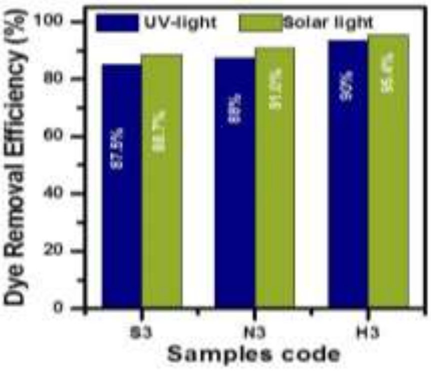
Environmental pollution has been a global issue; especially, water pollution is one of the main problems in the world that affects various sectors such as animals, plants and human beings, etc. Mostly organic pollutants are the primary sources for contamination of the water due to their toxicity and non-biodegradability. Photocalytic degradation is one of the best methods for the industrial effluent treatment. We have successfully synthesized TiO2 nanomaterial by various chemical methods like Precipitation, Microwave and Hydrothermal method. The prepared TiO2 nanomaterial was characterized by using various techniques such as XRD, FTIR, SEM, TEM and UV-DRS analysis. The photocatalytic activity of TiO2 nanomaterial was studied by the decolourization of methylene blue dye (MB) under UV and solar light irradiation. The maximum dye removal efficiency of 95 % was achieved under solar light irradiation. Thus, titanium dioxide has most promising nanomaterial for practical application.

Key words: Pollution, Nanomaterial, Photocatalytic degradation, TiO2



6.6 Accumulation of Heavy Metals in The Sediments of Karankadu Mangrove, Palk Bay, Southeastern India

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The mangrove forest is one of the most important components of marine environment, which is rich in biodiversity and ecosystem. In the present study, heavy metals (Zn, Cu, Pb, Cd) were analysed from 12 stations in the sediments of Karankadu mangrove in Palk bay region of south-eastern India. Among which the Zn concentration varied between 3.7±0.01 ppm to 14.2 ± 0.00 ppm. Then the concentration of Cu ranged from 1.44 ± 0.01 ppm to 8.93 ± 0.01 ppm. The Pb concentration varied from minimum of 1.42 ± 0.00 ppm to maximum of 4.02 ± 0.00 ppm. Similarly, the Cd concentration ranged from 0.28 ± 0.00 ppm to 0.59 ± 0.00 ppm was observed. The order of heavy metal found in the sediment samples was Zn > Cu > Pb > Cd. The Cd levels are within the prescribed limits of National and International regulatory agencies.

7. Green Chemistry

7.1 Green Synthesis and Characterization of Silver Nanoparticles from Azadirachtaindica (Neem) Leaf Extract by Hydrothermal Method

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In comparison to chemical and physical approaches, the biosynthesis of nano silver is attractive because of its low cost and environmental friendliness. There are many uses for silver nanoparticles (AgNps) in the medical field. Azadirachtaindica is a plant that is employed in many traditional medicine applications due to its powerful therapeutic characteristics. This study employs a green, eco-friendly, and convenient hydrothermal method for the synthesis of stable silver nanoparticles (Ag NPs) using medically beneficial. Azadirachtaindica leaf extract contains flavonoids and terpenoids that act as reducing as well as capping agents. Careful optimization of hydrothermal conditions leads to the formation of spherical Ag NPs. The green synthesis of Ag nanoparticles (AgNPs) were prepared and characterized. The crystalline nature of agnates was confirmed using X-ray diffraction (XRD). The size of the AgNps was 84.8nm calculated using the scherrer formula. Energy dispersive X-ray spectroscopy (EDx) research on the chemical makeup and functionality of plant extracts and NPs revealed the compositional mass ratio. The scanning electron microscopy showed the spherical shape of the nanoparticles. The prepared Ag nanoparticles are non toxic, ecofriendly and economical.

Keywords: Green Synthesis, Silver Nanoparticles, Hydrothermal, Azadirachtaindica.

7.2 Studies on naturally derived sugar IL as a green catalyst for the effective synthesis of bioactive coumarin derivatives

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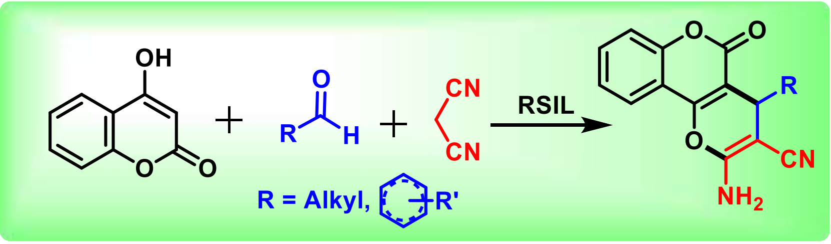
Abstract: 2-amino-3-cyano-4H-chromene derivatives were synthesised in a one-pot multi-component reaction using naturally derived sugar-based ionic liquid as a catalyst under mild reaction conditions. Natural carbohydrate was used as the sugar source for the formation of D-ribose-based sugar ionic liquid (RSIL). The catalyst RSIL was prepared in three steps. The synthesis of these ploy heterocyclic functionalized compounds involved two significant named reactions, namely the Knoevenagel condensation and the Michael addition reactions. A variety of substrates were synthesised using substituted aliphatic and aromatic aldehydes. The rate of reaction was unaffected by substitutions in the phenyl ring of benzaldehyde. The research findings will be presented in detail at the upcoming conference.



Highlights"
Metal Free synthesis
Mild reaction conditions
No Chromatography
Biological active molecules
No waste is generated

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7.3 Moringa oleifera seed extract based CS-Co_3O_4/MOE composite

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In current decades, metal oxide nanoparticles are generated through green chemistry methods being low cost, eco-friendly and non-toxic in nature. For an environmentally benign synthesis, plants seem to be the best candidates due to the presence of terpenoids, poly- phenols, alkaloids and phenolic acids which reduces the metal ions. Further, the

nanoparticles are incorporated into biodegradable polymer to elevate its antimicrobial properties. Cobalt oxide is a typical transition metal oxide having antibacterial, anticancer, antioxidant and antifungal properties. In this work, synthesis of Co3O4 Nps is done with the aid of Moringa oleifera (drumstick) seed extract. Then, the green synthesized Co3O4 Nps were well incorporated into chitosan matrix through co-precipitation method. The functional groups in the composite were identified using FTIR technique and the optical property was determined using UV-Vis spectra. XRD analysis examines the crystalline behavior of composite and HR-SEM images reveal the surface property of the prepared composite (CS-Co3O4/MOE). The antibacterial activity of the composite is then evaluated against selective Gram positive (S.aureus) and Gram negative (E. coli) bacterial species.

Keywords: Composite, CS-Co3O4/MOE, Antibacterial activity.

7.4 Promising antioxidant and anticorrosion properties of low carbon steel in 1M sulphuric acid solution by extract of Docynia indica

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Various parts of Docynia indica (D. indica) plant like leaf, root, stem and fruit were examined for their anti-corrosive property for low carbon steel (LCS) under 1M H2SO4. Total phenolic contents (TPC) and total flavonoid contents (TFC) of each part of plant was measured to ascertain the corrosion inhibition property. Weight loss, temperature studies and AAS were performed to determine the percentage of inhibition efficiency (IE%) by varying the concentrations from 50 to 250 ppm with an increment of 50 ppm. From these studies, leaf extract gave higher IE of 97.25% at 250 ppm concentration when compare to root, stem and fruit extracts. UV-visible, Fourier transform infrared (FT-IR), scanning electron microscopy (SEM), energy-dispersive x-ray spectroscopy (EDX) and atomic force microscopy (AFM) studies were performed for leaf extract with 250 ppm to confirm the corrosion inhibition characteristics of the D. indica plant extract. SEM and AFM studies substantiate with the images of the LCS validate the anticorrosive property of D. indica by forming protective film of phytochemical components on the metal surface.

Keywords: Docynia indica, Corrosion, Low carbon steel, SEM-EDX, AFM

7.5 Facile synthesis of CS-ZnO/AHE composite using Artocarpus heterophyllus seed extract

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The development of antimicrobial compounds has received more attention in recent years as a result of growing concern about bacterial and fungal contamination in health care and food industries. Recently, plants were employed for the preparation of metal oxide to minimize the consumption of toxic chemicals. Among various metal oxide nanoparticles, zinc oxide is often preferred due to its nontoxic nature and diverse physical, chemical and biological properties. Chitosan is a beneficial biopolymer and a powerful chelating agent that can form chemical bonds with transition metals results in better stability of composites. In the present study, ZnO was synthesized via simple co-precipitation method by using Artocarpus heterophyllus (jack fruit) seed extract and it is immobilized in chitosan matrix. The final composite is designated as CS-ZnO/AHE and characterized by UV-Vis, FT-IR and XRD analysis. The morphological features of the composite were investigated by HR-SEM analysis. The prepared nanocomposite is then used as an antibacterial agents tested against the Gram positive (S.aureus) and Gram negative (E. coli) bacterial pathogens.

Keywords: Composite, CS-ZnO/AHE, Antibacterial activity.

7.6 Vitis vinifera seed extract mediated synthesis of CS-MnO_2/VVE composite

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Nanotechnology is an emerging research areas of modern science and technology due to its multifunctional applications. Most of all, metal oxide nanoparticles have potential applications in various fields, mainly in biomedical sector. Recently, bio-inspired synthesis of

MnO2 NPs, especially using plants has received much attention being eco-friendly, low cost, and facile synthesis process. In the present investigation, synthesis of CS-MnO2/VVE nanocomposite is achieved by employing Manganese nitrate as initial agent and Vitis vinifera (grape) seed extract as reducing agent and chitosan as a capping agent. Chitosan, the second abundant naturally occurring polysaccharide is a biocompatible and biodegradable polymer that has been widely used in the preparation of metal oxide composites. The CS-MnO2/VVE composite was synthesized via co-precipitation method. The optical properties and nature of functional groups were studied by UV-Vis and FT-IR techniques. The crystalline nature and the morphological features of the composite were investigated by XRD and HR-SEM analysis. Finally, the antibacterial action of prepared nanocomposite is then tested against Gram positive (S.aureus) and Gram negative (E. coli) bacterial pathogens.

Keywords: Composite, CS-MnO2/VVE, Antibacterial action.

7.7 Preparation of CS-CuO/TGE composite by Trigonella foenum-graecum seed extract

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In the last few decades, metal oxide nanoparticles have been utilized in numerous fields of science and technology. The surface chemistry and size distribution of nanoparticles get altered after capping it with suitable biocompatible surfactants. In this work, chitosan due to its exceptional biological properties has attained significant focus in the biomedical field has chosen as a capping agent. Above all, Copper oxide nanoparticles [CuO NPs] have greatly researched nowadays as it displays enhanced antimicrobial activity towards pathogenic microorganisms. In the current study, we describe a greener method for producing stable chitosan embedded CuO NPs in which chitosan acts as a stabilizing agent, copper (II) nitrate as the precursor and Trigonella foenum-graecum (fenugreek) seed extract as a green reducing agent. The CS-CuO/TGE composite was synthesized through simple and effortless co-precipitation method. The prepared composite was then characterized using different spectroscopic techniques such as FT-IR, XRD, UV–Vis, and FE-SEM. Finally, Gram positive (S.aureus) and gram negative (E. coli) bacterial pathogens were used to test the effectiveness of the antibacterial property of the prepared composites.

Keywords: Composite, CS-CuO/TGE, antibacterial property.

7.8 Antibacterial effects of Pt Nanoparticles obtained from Plant Extract by Green Synthesis

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An eco-friendly and non-toxic chemical, Aerva lanata extract, was boiled and filtered to synthesize nanoparticles using a conventional green chemistry process. The aqueous Aerva lanata extract is used and it acts as a reducing and stabilizing agent, resulting in the reduction of platinum ions to platinum nanoparticles. The synthesis of platinum nanoparticles using plant extracts is a pricey process. This method can be used as an economical and biocompatible method. It can be described as a "simple green direction" because it does not require the organic solvents and expensive chemicals for developing platinum nanoparticles. At 80°C, the effect of temperature on platinum nanoparticles was studied. The formations of synthesized platinum nanoparticles were characterized by UV-Visible, X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). The platinum nanoparticles showed extremely powerful antibacterial activity in tests against harmful pathogens.

Keywords: Green synthesis, H2PtCl6, UV-Visible, XRD, FTIR and Antibacterial

7.9 Green synthesis of CS-ZrO_2/MIE composite via Mangifera indica seed extract

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At present, in order to minimize the consumption of toxic chemicals, various parts of plant extracts were used in the preparation of nanomaterials as reducing agent. Hence green synthesis becomes eco-friendly, economical, simple and safe for biomedical applications.

Moreover, a fresh interest in biocomposite has been sparked by the emergence of widespread bacterial infections. In the past few years, researchers have combined metal oxide nanoparticles and biocompatible chitosan to develop new hybrid composite. ZrO2 is a significant material having a large number of oxygen vacancies on its surface and a P-type semiconductor with a broad band gap. In this report, synthesis of zirconium oxide nanoparticles (ZrO2 Nps) chitosan composite (CS-ZrO2/MIE) is formulated by the aid of Mangifera indica (mango) seed extract. The mango seed kernels can serve as a perfect reducing extract comprising lot of bioactive components. The structural characterization and morphological features of the composite were studied by UV-Vis, FT-IR, XRD and HR-SEM analysis. Results from antibacterial test shows that CS-ZrO2/MIE composite is effective against gram negative (E. coli) and Gram positive (S.aureus) bacterial pathogens.

Keywords: Composite, CS-ZrO2/MIE, Antibacterial test.

7.10 Microwave Assisted Sustainable Synthesis of D-Glucose based Ionic Liquids: A Biocompatible Catalyst for Synthesis of Dihydropyrano Coumarins in Aqueous Media

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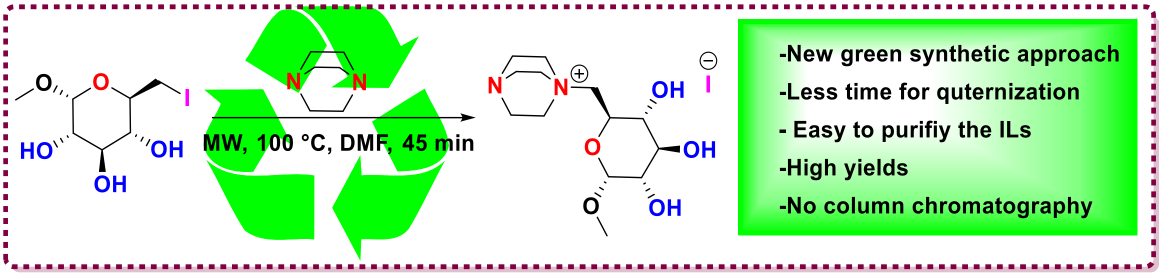
Herein, synthesis of DABCO based basic ionic liquid derived from D-glucose in excellent yields based on microwave assisted, simple three step approach. The advantage of the methods includes rapidness, convenience, eco-friendly, high atom economy, and excellent yields. The protocol should find wider application in synthesis of GIL in the future. This synthesized glucose based ionic liquids (GILs) were studied as a catalyst in multicomponent reactions for the synthesis of functionalized dihydropyrano coumarin derivatives in mild and green conditions. Developed GILs are biocompatible and exhibited excellent catalytic activity as well as good recoverability.



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7.11 Green synthesized Cobalt oxide Nanoparticles via Acalypha indica leaves extract and Sodium alginate Biocomposite Film for Atopic dermatitis Application.

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The current study aimed to evaluate the anti-inflammatory skin treatment (Atopic dermatitis) of green-synthesized cobalt oxide (CoO) nanoparticles using Acalypha indica leaves extract and Sodium alginate (NaAlg) biocomposite film. Cobalt acetate tetrahydrate as the precursor, and Acalypha indica leaves extract acts as the reducing agent. A simple co-precipitation method used to synthesis CoO NPs. The phytochemicals in leaves extract are essential for the production of CoO NPs. Recent developments in biopolymer-based materials highlights the effectiveness of polysaccharide alginate forms, primarily extracted and exhibits attractive properties such as being non-toxic, hydrophilic, and biodegradable. A solvent casting method is used for the preparation of (NaAlg/Acalypha indica-CoO NPs) novel biocomposite film, which is characterized by scanning electron microscopy (SEM), X-ray diffraction spectroscopy (XRD), and thermogravimetric analysis (TGA). Synthesized nanoparticles were characterized by (FT-IR) and UV-visible spectroscopy. Escherichia coli (E. coli) and Staphylococcus aureus (S. aureus) were used to test the composite's efficacy as a bactericide against gram-negative and gram-positive bacteria. The in-vitro biocompatibility and the efficacy of a polymeric material based on (NaAlg/Acalypha indica-CoO NPs) for inflammatory skin treatment(Atopic dermatitis). Thus, the new perspectives on using different compositions when creating a polymer material film that could enhance its application in biomedical field.

Keywords: Sodium Alginate; Acalypha indica leaves extract; Cobalt Oxide; Biocomposite film; Inflammatory skin treatment.

7.12 Facile Green synthesis of Vanadium (V) oxide nanoparticles using Daucus carota extract

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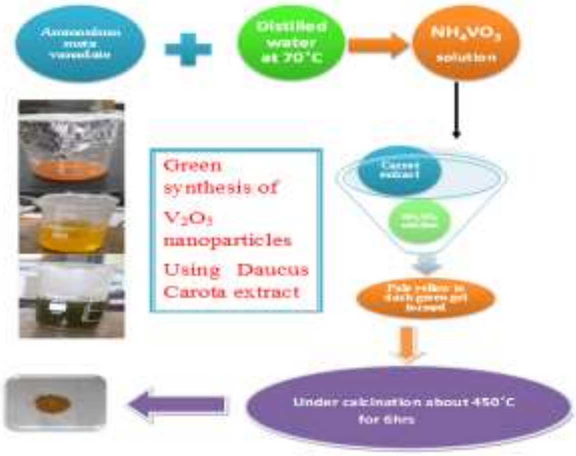
In this study, using Daucus carota (carrot) extract Vanadium Pentoxide ($V2O5$) has been prepared in a single inexpensive step. The dried dark green precursor xerogel was heated to 450˚C and left there for 6 hours. The obtained vanadium pentoxide nanoparticles were characterized using X-ray diffraction and Raman spectroscopic analysis. X-ray diffractometry results revealed that, the synthesized nanoparticles are to be in pure crystalline orthorhombic phase (001) and no other sub oxides of the metal oxide phases are noticed. Raman spectra analysis defined the layered structure of $V2O5$ nanoparticles and its crystalline defects are observed.



Key words: Green synthesis method, xerogel, nanoparticles, X-ray diffractometry, orthorhombic phase

7.13 CdO nanoparticles via Tridax procumbens green synthesis: Morphological, Spectral and Structural property

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Cadmium oxide (CdO) nanoparticles have been biosynthesized via Tridax procumbens leaf extract and characterized using different analytical techniques. XRD analysis indicated FCC structure with average crystallite size being 36.28 nm. It is well noticed that the synthesized CdO nanopowder using this Green method also exhibited a strong (1 1 1) preferential orientation. The Crystalline size (D), Microstrain (ϵ) and the Dislocation density (δ) were calculated using the Scherrer's formula. Morphological analyses involving SEM confirmed the cubic crystalline nature of the prepared samples. EDS spectrum recorded for the green synthesized nanopowder which confirms the presence of Cd and O peaks in the prepared sample. The presence of Cd-O bond was ascertained using FTIR technique.

Keywords: Tridax procumbens, cadmium oxide, FTIR and SEM-EDS

7.14 Studies on effective Zinc Oxide Nanoparticles via Acalypha indica leaves extract and Sodium alginate Biocomposite Film for Allergic contact dermatitis Applicaton.

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A type of natural material, Sodium Alginate, has been widely investigated and used in treatment of wound and skin burn management. The objective of this work is to assess the inflammatory skin treatment via green-synthesized ZnO NPs from Acalypha indica leaves extract, and Sodium alginate (NaAlg) biocomposite film. Acalypha indica leaves extract was used as a reducing agent and zinc chloride as a precursor in the co-precipitation method to synthesize zinc oxide NPs, the phytochemicals in leaves extract are essential for the production of ZnO NPs. A solvent casting method is used for the preparation of (NaAlg/Acalypha indica-ZnO NPs) novel biocomposite film and characterize by scanning electron microscopy (SEM), X-ray diffraction spectroscopy (XRD), and Thermogravimetric analysis (TGA). Synthesized nanoparticles were characterized by (FT-IR) and UV–Visible spectroscopy. Escherichia coli (E. coli) and Staphylococcus aureus (S. aureus) were used to test the efficacy of biocomposite film as a bactericide against both gram-negative and gram-positive bacteria. The in-vitro biocompatibility and the efficacy of a polymeric material composite based on NaAlg and green-synthesized ZnO NPs from Acalypha indica leaves extract complex for anti-inflammation (Allergic contact dermatitis). A biocomposite film made of NaAlg/Acalypha indica-ZnO NPs reduces the inflammatory response. Thus, the cost-effective NaAlg/Acalypha indica-ZnO NPs film obtained through green-synthesis method for their potential applications in the field of biomedical applications.

Keywords: Zinc Oxide; Acalypha indica leaves extract; Sodium Alginate; Biocomposite film; Inflammatory skin treatment.

7.15 Carica papaya seed extract assisted synthesis of CS-MgO/CPE composite

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Currently, bio-polymer based MgO nanocomposites has received center of interest in the biomedical and pharmaceutical sectors due to its nontoxicity and biodegradability. Magnesium oxide is a versatile compound due to its unique optical, mechanical, chemical, electrical properties. Chitosan (CS), a beneficial biopolymer is widely researched owing to its special features including biocompatibility, chelating ability and antimicrobial activity. Biological synthesis or green synthesis is an efficient approach avoiding harsh conditions and not utilizing hazardous chemicals. The phytochemical constituents in the seed extract results in successful reduction of metal ions and the combined effect of chitosan and metal oxide elevates the bactericidal effect predominantly. Herein, synthesis of CS-MgO/CPE composite is achieved by simple chemical precipitation method with magnesium nitrate as a source material, Carica papaya seed extract as a reducing agent and chitosan as a stabilizing agent.

Then the structural, morphological and functional properties were characterized by UV-Vis, FT-IR, XRD and HR-SEM analysis. The prepared nanocomposite had an efficient antibacterial activity towards the Gram positive (S.aureus) and Gram negative (E. coli) bacterial pathogens.

Keywords: Composite, CS-MgO/CPE, Antibacterial activity.

7.16 Incorporation of green synthesized ZnO on chitosan matrix and evaluating its antimicrobial and antioxidant potential

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Nanocomposites are the mixture of heterogeneous materials comprising biopolymer and inorganic metal oxide exhibits exceptional features that appropriate for various biomedical applications. Green synthesis of chitosan based nanocomposites are broadly researched as it is simple, cost-effective, biocompatible and eco-friendly procedure. The present study aims to examine antimicrobial and antioxidant potency of chitosan embedded zinc oxide nanocomposite prepared using Cissus quadrangularis plant extract as a green reducing agent. Chitosan acts as a suitable template and phytochemicals in the plant reduce the metal salts naturally forming stable chelates. Moreover, the optical properties, nature of functional groups and thermal stability of the prepared samples were analysed by UV-Vis, FT-IR, and TGA analysis. The crystalline nature and morphological features of the composites were confirmed through XRD and HR-SEM techniques. XPS and BET studies evaluate the electronic state and specific surface area. These results evidently elucidates the effective formation of CS-ZnO/CQE nanocomposite. Subsequently, the bacteriostatic along with fungicidal effects of the nanocomposite is then investigated via agar well diffusion method against S. aureus, E. coli bacterial pathogens and A.ochraceus, A. niger fungal strains. The free radical scavenging ability was determined by DPPH assay.

Keywords: Nanocomposite, CS-ZnO/CQE, antimicrobial, antioxidant.

8. Nanotechnology

8.1 Precision Nanocluster-Based Toroidal and Supertoroidal Frameworks Using Photocycloaddition-Assisted Dynamic Covalent Chemistry

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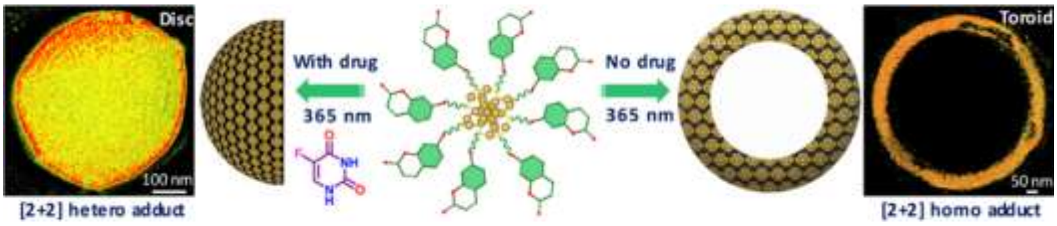
Ligand-protected atomically precise nanoclusters derived from coinage metals are ideal building blocks to construct self-assembled superstructures. Though photon-assisted supramolecular reversible self-assembly in precision nanoclusters has been reported, long-range self-assembly based on classical photochemical reactions on the nanocluster surface has yet to be investigated. Herein, we present the synthesis and light-induced reversible self-assembly of coumarin tethered Au25 nanoclusters via [2+2] photocycloaddition reaction. Photoactivation of functionalized nanoclusters dispersed in tetrahydrofuran results in the formation of uniform toroidal superstructures. The mechanism of toroidal formation and the influence of long-term lighting on the structural rearrangement of toroids have been investigated. High-resolution transmission electron microscopy, electron tomographic reconstruction, atomic force microscopy, and field-emission scanning electron microscopy results suggest that toroids are made up of densely packed nanoclusters. Prolonged illumination of nanoclusters under 365 nm light results in the formation of honeycomb frameworks due to the inter-structural coupling between the adjacent toroids. Finally, we demonstrate the fabrication of a "model-smart drug delivery system" by employing a cross-photocycloaddition reaction between coumarin-tethered nanoclusters and an anticancer drug (5-fluorouracil). The formulated nanocluster-based molecular device shows systematic loading and unloading of the drug during the assembly and disassembly under two distinct windows of light. Such systems with appropriate modifications will be an ideal probe for addressing noninvasive drug delivery and theranostics in the future.



8.2 Synergistic effect in α-Fe_2O_3 - Chitosan Nanocomposite with enhanced Adsorption of Methyene Blue Dye

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In this work, we synthesize the α-Fe2O3-Chitosan nanocomposite using co-precipitation method. Structural and surface morphology of nanocomposite is investigated using XRD, and SEM. Further characterizations are performed using UV-Visible and FTIR Spectroscopy, photoluminescence and EDX. The average crystalline size of nanocomposite α-Fe2O3-Chitosan nanocompositeis is 25.8 nm. Elemental composition of the prepared samples was confirmed by EDX spectrum. The prepared nanocomposite is proposed as a potential material for higher dye adsorption. The Fe2O3-Chitosan nanocomposite could remove methylene blue (MB) as a cationic dye from waste water corresponding to second-order kinetic model. Thermodynamic studies showed that adsorption equilibrium constant (KL) and maximum adsorption capacities (Qmax) were increased with increasing temperature. The removal efficiency of MB for Co 0.01 mmol/L at optimum conditions was about 90%. The maximum uptake capacity (Qmax) of methylene blue in a batch reactor was 0.3, 0.5 and 0.7 mmol/g at 15, 25 and 40 °C, respectively.

Keywords: Chitosan, α-Fe2O3 NPs, Nanocomposite,Methylene Blue, Adbsroption

8.3 Biosynthesis of Zinc Oxide nanoparticles from cyanobacteria (Microsiera Wollies) and their anticancer activity against human A549 lung cancer cells

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Lung cancer is a major cause of cancer-related death worldwide, with a very poor survival rate. The limitations associated with the conventional diagnosis and therapeutic strategies used for lung cancer have motivated the development of nanotechnology and nanomedicine approaches, in order to improve early diagnosis rate and develop more effective and safer therapeutic options for lung cancer. Cancer nanomedicines aim to individualize drug delivery, diagnosis, and therapy by narrowing them to each patient's unique physiology and pathological feature on both the genomic and proteomic levels and have attracted widespread attention in this field. Despite the successful application of nanomedicine techniques in lung cancer research, the clinical translation of nanomedicine approaches remains challenging due to the limited understanding of the interactions that occur between nanotechnology and biology, and the challenges posed by the toxicology, pharmacology, immunology, and largescale manufacturing of nanoparticles. Synthesis of Zinc Oxide nanoparticles (ZnO NPs) by an ecological approach using cyanobacteria (Microsiera wollies) as reducing agent was carried out. ZnO NPs was synthesized from aqueous zinc chloride solution by cell-free supernatant of a novel isolate. Hyperchromic shift was observed at 364 nm using UV–Visible spectroscopy, The presence of functional molecules was confirmed by Fourier Transform Infrared spectroscopy (FTIR) and X-Ray Diffraction (XRD). The surface morphology was analyzed and confirmed by Scanning Electron Microscopy. In this work, we highlighted the progress and opportunities associated with Zinc Oxide nanoparticles against lung cancer and discussed its prospects, together with the challenges associated with clinical translation. The anti-cancer activity of the ZnO NPs was carried out using ZnO as a drug against A549 lung cancer cell.

Keywords: Lung cancer, cyanobacteria, Microsiera wollies, Nanomedicine, Anti-cancer

8.4 Shell-isolated Nanoparticle Enhanced Raman Spectroscopy (SHINERS): A Versatile Tool for Probing Electrochemical Reactions

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Investigating the behaviour of the analytes at the electrode surface is crucial in understanding the electrochemcial and elctrocatalytic reactions. Ther are several analytical techniques has been developed to itenditify the interface mechanisms in electrochemcial process. Among that, Raman spectroscopic technique is an non-destructive tool for obtaining vibrational spectral information about the surface species and helpful in investigating the in-situ electrochemcal reactions. Though Raman signals are very week, corrugated metal surfaces greatly enhance the Raman signal by several orders of magnitude and it is belived by means of electromagnetic and chemical enhancement theories. This methodoloy is termed as Surface-Enhanced Raman Spectrocopy (SERS). Using the shell isolated core metal nanoparticles prevent the chemical interaction and enhance the Raman signal only in the terms of electromagnetic mode and this is called as Shell-Isolated Nanoparticle Enhanced Raman Spectroscopy (SHINERS). Here, at first, we demonstrated the unintentional catalytic interference from silver nanoparticles in spectroelectrochemical studies and its mitigation using thin pinhole-free silica layer covering the silver nanoparticle (Ag@SiO2). And secondly, the application of SHINERS is employed to probe the transient potential behavior of self-organized systems which involves a sequence of mass transfer limited chemical reactions. Our studies show the advancement of Raman spectroscopy in the field of electrochemistry, where it might be crucial in comprehending the underlying principles of any electrochemical reactions. We anticipate that the observations from this study would help SHINERS to gain more visibility among global researchers working on fundamental electrochemistry challenges such as batteries, catalytic water splitting reactions and more.

Keywords: Raman spectroscopy; SERS; SHINERS; electrochemistry; charge-transfer; interference.

8.5 Preparation of Liposomes from Egg Lecithin

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This investigation presents a method to prepare liposomes for egg lecithin. Egg yolk is an excellent source of phospholipids. Egg yolk powder (EYP) contains about 60% lipids, which consist of, on average, neutral lipids (65%), phospholipids (31%), and cholesterol (4%). A Phospholipid is composed of a glycerol backbone attached to one and two fatty acids and other ends esterified phosphoric acid and the organic alcoholic group. The isolation of high-purity egg yolk phospholipids. Phospholipid was characterised by UV and FTIR spectroscopy. Then prepared, liposome by thin film hydration method. The liposome was studied for its stability and size. Then natural extraction is injected into the liposome. Phospholipid-based liposomal vesicles are among the most effective delivery options for various diseases. The applications of phospholipids in drug delivery systems are the enhancement of bioavailability of drugs with low aqueous solubility or low membrane penetration, an improvement or alteration of the uptake and release of the drug, and protection of sensitive active agents from degradation. Liposomes deliver both hydrophilic and hydrophobic drugs for cancer, antifungal, antibacterial, immunomodulation, diagnostics, ophthalmia, vaccines, enzymes, and genetic elements.

keywords: Phospholipid, egg yolk phospholipid, liposomes, natural extraction, and drug delivery.

8.6 Preparation and Characterization of CG-ZnO nanocomposite and evaluation in photodegradation of methylene blue dye.

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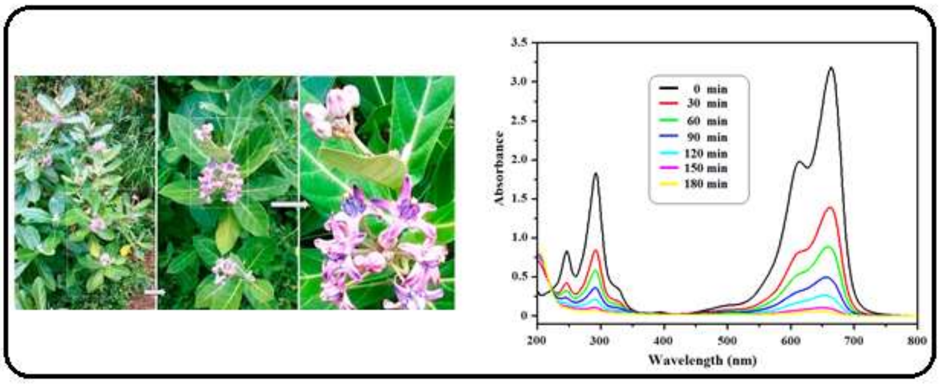
The present work reports the preparation of Calotropis Gigantea doped ZnO nanocomposite (CG-ZnO) by co precipitation method. The nanocomposite demonstrated excellent selectivity and was used for the removal of toxic cationic methylene blue dye (MB). The synthesized nanocomposite were characterized with UV-Visible, FRIT, XRD, FESEM and BET analysis. The absorption peaks appeared at 284 and 282 nm which is attributed to the presence of CG on ZnO. The FT-IR analysis the peak at 1570 cm-1 -NH stretching vibration of CG and 421,423 and 438 which is attributed to the ZnO stretching vibration. The XRD

pattern revealed that the nanocomposite are crystalline in nature. The flower like morphology and porosity of CG-ZnO were confirmed using FESEM and BET respectively. The photocatalytic activity of CG-ZnO nanocomposite was investigated under the direct sunlight irradiation. The CG-ZnO nanocomposie showed good chemical stability, reusability and 92% of was removed within 180 minutes.

Keywords: Calotropis Gigantea, ZnO, FESEM, Methylene Blue, Photodegradation



8.7 Preparation and Characterization of CG-ZnO nanocomposite and evaluation in antibacterial activity.

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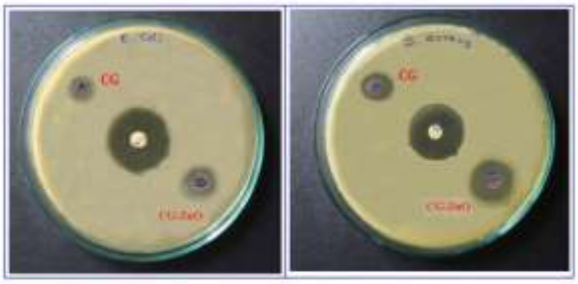
The present work reports the preparation of Calotropis Gigantea doped ZnO nanocomposite (CG-ZnO) by co precipitation method. The nanocomposite demonstrated excellent selectivity and was used for the removal of toxic cationic methylene blue dye (MB). The synthesized nanocomposite were characterized with UV-Visible, FRIT, XRD, FESEM and BET analysis. The absorption peaks appeared at 284 and 282 nm which is attributed to the presence of CG on ZnO. The FT-IR analysis the peak at 1570 cm-1 -NH stretching vibration of CG and 421,423 and 438 which is attributed to the ZnO stretching vibration. The XRD pattern revealed that the nanocomposite are crystalline in nature. The flower like morphology of CG-ZnO were confirmed using FESEM. Finally, the antibacterial activity of the prepared CG-ZnO nanocomposite was tested against Gram-Positive and Gram-Negative. The maximum zone of inhibition was observed for Escherichia coli than Staphylococcus

aureus.With the above results, we suggest that the prepare nanocomposite serve as better antibacterial agent.

Keywords: Calotropis Gigantea, ZnO, FESEM, Disc diffusion method, Antibacterial activity.



8.8 Synthesis of Mg-doped copper oxide nanorod using co-precipitation method: their physicochemical and antimicrobial properties

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Abstract Last two decades, various antibacterial strategies have been made possible by synthesizing nanomaterials (NMs). Continuous treatment of nanoparticles against bacteria leads to the strains has gains resistance against nanoparticles. To overcome this issue, researchers believed that the doping method could enhance the antibacterial activity of metal oxide nanoparticles. According to this objective, in the current study, magnesium ions were doped in the copper oxide nanorods (Mg-CuO NRs) by the co-precipitation method. PEG was used as the capping agent. The as-prepared sample [Mg-Cu (OH)2] was calcined at 500°C for 4h. Synthesized Mg-CuO NRs were characterized by TGA, UV-Vis-DRS, FTIR, Raman, PL, ZP, XRD, and FE-SEM with EDAX elemental mapping, TEM, and XPS analysis. Different concentrations of synthesized Mg-CuO NRs (0.5, 1, 2 mg) were tested against microorganisms of Bacillus megaterium, B. subtilis, Shigella dysenteriae, and Candida albicans. The antimicrobial activity of the Mg-CuO NRs revealed the activity in was dose-dependent manner. Initially, Mg-CuO NRs contact the bacteria by electrostatic interaction. As a result, it produced surface tension that generated dual ions, releasing the ability of

Mg2+ and Cu2+ ions and promoting bacterial cell wall structural integrity loss. This material can potentially be used in the near future for anti-biofilm coating, photothermal therapy, the manufacture of bio-implant materials, and polymer coating to enhance mechanical qualities.

Keyword: Doping, Nanorods; Mg2+ ion, Cu2+ ion; Electrostatic interaction, Ions releasing

9. Photocatalysts

9.1 Synthesis of direct Z-scheme $FeMoO_4$/g–C_3N_4–2D/2D heterojunction photocatalyst for water treatment

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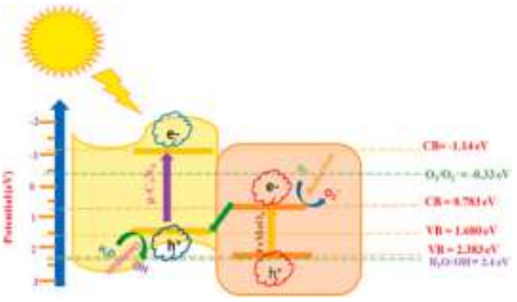
In this work, we synthesised FeMoO4/g-C3N4-2D/2D Z-scheme heterojunction photocatalyst by wet chemical method and characterized through X-ray diffraction, FT-IR, UV–visible diffuse reflectance spectroscopy, scanning and transmission electron microscopy and photoluminescence techniques to confirm g-C3N4 was successfully loaded on the surface of FeMoO4. The photocatalytic activity of the synthesised FeMoO4/g-C3N4 composites were studied via the degradation of Rhodamine B (RhB) under visible light irradiation (VLI). The optimal FeMoO4/g-C3N4 composite showed an enhanced degradation performance with rate constant value of 0.02226 min–1 and good stability even after three cycles. The radical scavenging studies revealed that the h+and O2•—are the active radicals in the degradation of RhB under VLI. It is proposed that the FeMoO4/g-C3N4 formed a Z-scheme heterojunction effectively thereby enhanced the transfer and separation ability of e-/h+pairs. Thus, the newly constructed Z-scheme FeMoO4/g-C3N4 heterojunction photocatalyst is a promising material for the purification of wastewater to save the environment.

Keywords: FeMoO4/g-C3N4, Photocatalyst, Rhodamine B, Visible light, Wastewater treatment .



9.2 Photocatalytic Degradation of Pyrogallol Over TiO_2-Advanced Oxidation Process

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The degradation of Pyrogallol is approved out under UV-visible light by TiO2 as a photocatalyst. In the direction of determining the efficiency of the photocatalyst, the, unlike variables, studied built-in the amount of photocatalyst, consequence of oxidants peroxomonosulphate (PMS) and peroxodisulphate (PDS) on the photocatalytic oxidation of Pyrogallol on elucidation TiO2 surface have been investigating. The efficiencies of these oxidants on photocatalytic degradation of Pyrogallol are compared with that of PMS and PDS. The investigational results indicate that these oxidants reveal improved rates of mineralization of Pyrogallol. A response mechanism, linking the production of hydroxyl radicals and sulfate radicals. In conclusion, this investigation indicated a high potential of TiO2 suspension to remove the high-level concentration of Pyrogallol under UV radiation.

Keywords: Photodegradation, Pyrogallol, PMS, PDS, TiO2 Catalyst.

9.3 The photocatalytic study analysis on Polyprrole/Zinc Oxide nanocomposite towards the degradation of methylene blue under sunlight

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This study reports the structural, optical, morphological, and photocatalytic analyses of polypyrrole/zinc oxide nanocomposite (Ppy/ZnO NC) synthesised by in-situ polymerization.The synthesized samples are characterised by powder X-ray diffraction (PXRD), field emission scanning electron microscopy (FE-SEM), and diffuse reflectance UV-Vis spectra. It is also being studied for the photo-degradation of methylene blue in direct sunlight. The XRD pattern showed that the ZnO in the nanocomposite has a polycrystalline hexagonal wurtzite structure with no extra phases and an average particle size of 17.1 nm. FE-SEM images demonstrated the nanowarm-like morphologies of Ppy/ZnO NC. The reflectance band edge exhibited a low reflectance (%) in the entire visible region and a band gap value of 2.3 eV calculated from the Kubelka-Munk relation. The photocatalytic activity of the prepared nanocomposite was employed for the photodegradation of methylene blue and exhibited a maximum efficiency of 95% in a period of 60 minutes.

Keywords: Photocatalytic acivity; Methylene blue ;FESEM; polymerization technique

9.4 Development of visible light photocatalyst for removal of reactive dyes

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Titanium dioxide (TiO2) is a nontoxic material and has been applied in environmental treatments such as water and air purification, water disinfection and sterilization because of its unique properties such as strong photocatalytic activity and chemical stability. The most widely accepted mechanism is the migration of valence electron to conduction band and the formation of electron-hole pairs. These electron-hole pairs react with adsorbed molecules at semiconductor surface, resulting in the degradation of adsorbates. The only drawback of using TiO2 is that it has wide band gap energies (3.2eV) and its activity in UV region. There is a need for efficient visible light photocatalyst which can enhance and promote catalytic process under sun. Considerable effort has been focused on the development of composite material for photocatalytic activity on the effluent treatment. Generally, polymers are synthetic materials; their biocompatibility and biodegradability are much more limited than those of natural polymers such as cellulose, chitin, chitosan and their derivatives. Chitin and chitosan are recommended as suitable functional materials because these natural polymers have excellent properties such as biocompatibility, biodegradability, non-toxicity, adsorption properties, etc. Chitosan is a natural carbohydrate biopolymer derived by N-deacetylation of Chitin (a linear polymer of N-acetyl-2-amino-2-deoxy-D-glucopyranose units with ß-(1-4) bonds) a major component of the shells of crustacean such as crab, shrimp and crawfish.

TiO2-chitosan composite was successfully prepared and well characterized. The formation of composite was confirmed by UV-Visible absorption spectra and the band gap was calculated using reflectance spectra. FT-IR analysis confirms the formation of the TiO2 and chitosan in the synthesized nanocomposite. The XRD confirms the tetragonal structure and phase purity of the sample. The morphology of TiO2-chitosan shows the particles are in the nanometer scale. The photocatalytic activity of the composite was evaluated for reactive dyes under visible light. Maximum percentage of degradation was achieved for the reactive dyes under visible light irradiation.

9.5 Morphology Dependent Photocatalytic Efficiency of nano ZnO for Water Purification

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In this work, we have successfully synthesized ZnO nanoparticles with three different morphologies in 1D, 2D and 3D respectively that are the rod, the wall and the sphere by using cost effective and chemical precipitation method. The formed ZnO samples were characterized using XRD, UV-DRS, SEM and BET techniques. XRD analysis confirmed the formation of ZnO in wurtzite structure in the all three samples. The morphologies were confirmed by the SEM analysis. The surface area of the formed ZnO nanoparticles were estimated from the BET results. Moreover, the photocatalytic activity of the ZnO nanoparticles against Azure A dye was examined by using UV-Visible spectrophotometer. Among the three samples, the nano spherical ZnO showed a high photocatalytic degradation rate.

9.6 A facile strategy to preparation of ZnO, Cu^{2+} - ZnO and Co^{2+} - ZnO nanoparticles with superior catalytic reductive degradation behavior under methylene blue via wet-chemical process

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Present work, green approach of ZnO, Cu2+ - ZnO and Co2+ - ZnO nanoparticles were synthesized using STL extract as reducing as well as stabilizing agents. The obtained samples were characterized using different approaches as XRD, FT-IR, SEM-EDX, UV-visible and BET measurements were used for the structural, morphological, and optical properties in nanoscale region. The cubic phase with the particle size were observed as 30-40, 22-30 and 10-20 nm, respectively by XRD and SEM analysis. In addition, the percentage degradation were found to be 63.5 %, 82.5 %, and 93.8 %, within 120 min of UV light irradiation using MeB in the presence of ZnO, Cu2+ - ZnO and Co2+ - ZnO respectively. Moreover, the pseudo-first order reaction rate constants were found to be 0.00298 min-1, 0.00345 min-1 and 0.00365 min-1 respectively. Among catalyst results, Co2+ - ZnO particles enhanced highest capability to photo- degrade the pollutants as MeB due to the generation of heterojunction interface among individual constituents. Consequently, it can be anticipated that Co2+ - ZnO particles could be used as multifunctional photocatalyst for the treatment of different environmental pollutants.

Keywords: ZnO; Cu2+ - ZnO; Co2+ - ZnO NPs; STL extract; Optical; Catalytic

9.7 Photocatalytic Performance of g-C_3N_4/WO_3 Nanocatalyst for the Organic Dye Degradation for Waste Water Treatment

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Photocatalysis holds great promise as an efficient and sustainable oxidation technology for application in wastewater treatment. Rapid progress in developing novel materials has propelled photocatalysis to the forefront of sustainable wastewater treatments. In this work, g-C3N4 /WO3 nanocomposite as photocatalyst was constructed by physical grinding of g-C3N4 and WO3. The as-synthesized photocatalysts were characterized by X-ray powder diffraction, Fourier transform infrared spectroscopy, UV–vis diffuse reflectance

spectroscopy, SEM, and photoluminescence. The photocatalytic activity of the photocatalyst was evaluated by degradation of Methylene Blue (MB) dye under a 300 W visible lamp. Compared to WO3 and g-C3N4, the g-C3N4 /WO3 composite exhibits an enhanced photocatalytic activity. The enhanced performance of g-C3N4 /WO3 composite photocatalyst was mainly ascribed to the effect between WO3 and g-C3N4, which improved the photogenerated carrier separation.

Keywords: Photocatalysis, Methylene Blue (MB), photogenerated carrier separation.

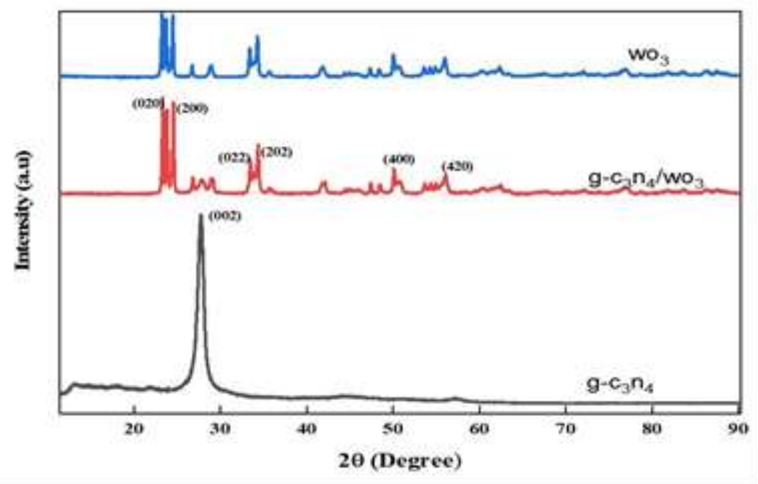

Figure 1: Comparison between the measured XRD pattern of g-C3N4, WO3, and g-C3N4/WO3 composite synthesized via physical grinding for 2 h and heated at 500°C.

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9.8 Synthesis and Characterization of g-C_3N_4/CeO_2 Nanocomposite and their Photocatalytic Performance for Wastewater Treatment

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In this work, we have studied the photocatalytic activities of the graphitic carbon nitride/cerium oxide (g-C3N4/CeO2) for methylene blue (MB) dye degradation under visible spectra. The g-C3N4/CeO2 photocatalyst was successfully prepared by simply mixing and grinding g-C3N4 and CeO2 followed by calcination. All prepared samples g-C3N4, CeO2 and g-C3N4/CeO2 were characterized via X-ray diffraction, FT-IR, photoluminescence, and UV-Visible absorption spectroscopy. The Photocatalytic activities of the prepared samples were examined by studying the degradation of methylene blue (MB) under visible light irradiation (>400 nm). g-C3N4 is a semiconductor polymeric photo-nanocatalyst used in dye degradation and water splitting process. It has excellent visible-light absorption, and high chemical & thermal stability and low recombination energy making it a better material for electron transportation. CeO2 exhibits high photocatalytic activity. The photocatalytic activity of CeO2 can be enhanced by modification in the morphology via doping with non-metal dopants and coupling with other semiconductors. The g-C3N4/CeO2 composite has shown higher photocatalytic activity (% DE = 93%) than individual C3N4, and CeO2. The optimum photo-activity of g-C3N4/CeO2 exhibited an improved photodegradation in pollutant treatment due to enhanced photocurrent under visible light., which is attributed to the synergetic effect between the C3N4 and CeO2.

Keywords: Photocatalysis, g-C3N4 /CeO2, Methylene Blue (MB), photogenerated carrier separation.

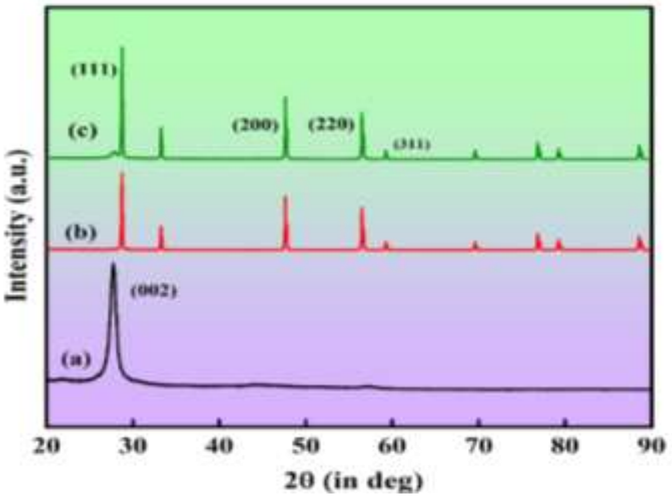

Figure 1: XRD pattern of (a) g-C3N4, (b) CeO2, and (c) g-C3N4/CeO2 composite prepared via physical grinding

References:

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9.9 Metal Oxide Graphene Nanocomposites for Organic and Heavy Metal Remediation

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In the research work, the main focus is to understand the structure and photocatalytic activity of titanium dioxide with graphene (G-TiO2) which is synthesized by using sol–gel method. The photocatalytic activity of TiO2 is limited by the short electron hole pair recombination time. Graphene, with high specific surface area and unique electronic properties, can be used as a good support for TiO2 to enhance the photocatalytic activity. The obtained G-TiO2 photocatalysts has been characterized by X-Ray Diffraction (XRD), Raman Spectroscopy, Transmission Electron Microscopy (TEM), FTIR Spectroscopy and Ultraviolet visible (UV-vis) Spectroscopy. The primary objective of the second work is to understand the nanocomposite structure of SiO2 coated over graphene (G) nanoplatelets. An attempt has been made to synthesize G-SiO2 nanocomposite using sol-gel technique. The G-SiO2 nanocomposite is characterized using Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Raman spectroscopy, FTIR spectroscopy, and Electrochemical and Electrical measurement technique, respectively. The presence of heavy metal is tested using electrochemical cyclic voltammetry (CV) technique. The CV measurement on the water treated with G-SiO2 has been tested for several days to understand the presence of heavy metals in water. Interestingly, the near complete separation has been observed by treating the heavy metal contaminated water sample for one to two days in presence of G-SiO2 nanoparticles. The redox potential observed for the heavy metal has been found to diminish as a function of treatment with respect to time, and no redox peak is observed after the treatment for four to five days. Further test using EDS measurement indicates that the heavy metal ions are observed within the G-SiO2 nanocomposite. The recovery of G-SiO2 nanocomposite is obtained by washing using deionized water. Our experimental finding indicates that the G-SiO2 nanocomposite could be exploited for potential heavy metals cleaning from waste or drinking water.

Key words: Metal oxide grapheme, Nanocomposites, Heavy metals, Environmental Remediations.

9.10 Synergistic effect of chitosan-ZrO_2-plectranthus amboinicus composite for antibacterial and photocatalytic activities

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In current scenario, metal nanoparticles have gained more attention in many fields due to their unique interaction with biomaterials. The present work describes a new biopolymer based CS-ZrO2-PLE composite was successfully synthesized by simple precipitation method. Presence of reactive functional groups in the chitosan and phytochemicals such as thymol, carvacrol, p-cymene, β-caryophyllene, α-pinene, β-pinene, 1,8-cineole etc in the plectranthus amboinicus leaf extract plays a major role in the stabilization of the CS-ZrO2-PLE composite. As synthesized composites optical property was studied by UV-Vis DRS spectroscopy. The chemical bonding and crystalline behaviors were confirmed by FT-IR and XRD analysis. The surface morphology of the biopolymer connected with ZrO2 particles confirmed by HR-SEM analysis. TGA results showed that these composites are thermally more stable. All the synthesized materials were tested for antibacterial activity. The CS-

ZrO2-PLE composite exhibited strong antibacterial activity against gram positive, Staphylococcus aureus (S.aureus) as well as gram negative, Escherichia coli (E.coli) microorganisms. Photocatalytic activities of synthesized composites have been evaluated with two different dyes (methylene blue and drimarene red). The photocatalytic degradation efficiency of CS-ZrO2-PLE composite was significantly improved.

Keywords: Chitosan, Plectranthus amboinicus, Antibacterial activity, Photocatalytic activity.

9.11 Photocatalyst Assisted Removal of Organic dye In Aqueous Media

By Low Cost Adsorbents

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The adsorption studies are of great significance to evaluate the adsorption performance for removal of coloured organic substance from aqueous media. Adsorption is one of the most widely applied technique where molecules tend to concentrate on the surface of the absorbent as a result of weak van der Walls forces of interaction between the molecules. The present study reports the removal of colored organic substance from aqueous solution using absorbent with photocatalyst. Adsorption experiments were carried out by varying parameters viz contact time, dosage of absorbent, substrate concentration and pH. The results revealed that Langmuir & Freundlich models provide better correlation for the replicate measuremental data, obeys first order kinetics and also observed maximum percentage adsorption. Furthermore electronic absorption and scanning electron microscopic analysis for the sample are under progress.

10. Polymer Chemistry

10.1 A polyrotaxanated covalent organic polymer based on viologen and cucurbit[7]uril

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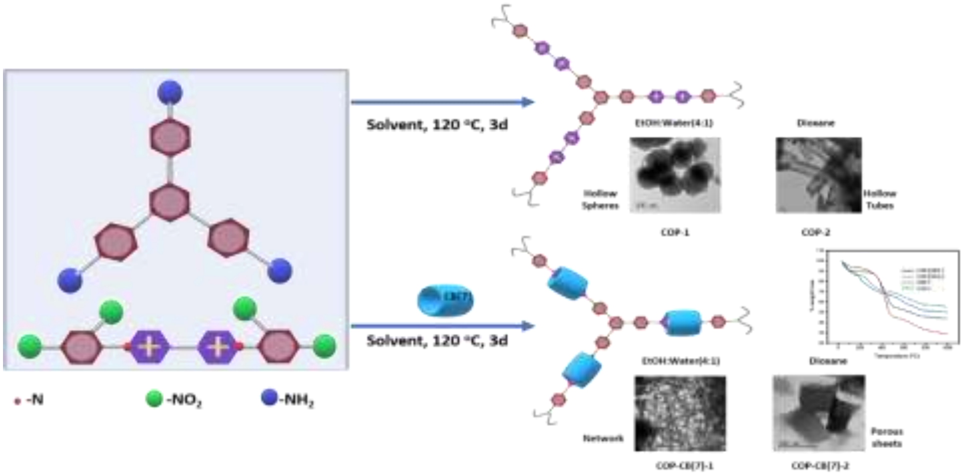
Insoluble and porous covalent organic polymers have gained recognition recently for their large surface areas' favourable capacity to engage in noncovalent interactions with other molecules. In the areas of gas separation and storage, pollutant abatement, catalysis, energy conversion, and sensing, this characteristic is particularly helpful. In light of all the impacts that the mechanical link has on the chemical and physical properties of materials, the immobilisation of mechanically interlocked molecules, such as rotaxanes, catananes, or knots into polymeric materials, became an interesting research subject. Here, we describe the synthesis of two distinct covalent organic polymers (COPs) based on viologen, COP-1 with a hollow sphere and COP-2 with a hollow tube morphology, as well as two distinct polyrotaxanated COPs based on viologen and cucurbit[7]uril, COP-CB[7]-1 with a network-like morphology and COP-CB[7]-2 with a porous sheet morphology, which were synthesized via the Zincke reaction by altering the polarity of the solvent. Comparisons are made between COPs that have been polyrotaxanated and those that haven't. The CB[7]-encapsulated polymer is more resistant to mechanical and thermal stresses. The synthetic approach described here enables the insertion of mechanically interlocked molecules into polymeric materials and opens the door to materials with yet-unknown characteristics and functions.



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10.2 Development and Characterization of Superabsorbent Fibre from Biopolymer Blend

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In current circumstance, textile fibers are used for wide range of applications such as clothing, geo textiles, agro-textiles and medical textiles etc. Development and consumption of textile fibers are proliferated day by day in the medical field. Especially, textile fibers have reasonable growth in hygiene products like napkin, diaper and incontinence pads. The currently used sanitary napkins contain synthetic superabsorbent polymer (SAP) granules which is a key component of the product. This synthetic superabsorbent polymer takes nearly 500 - 800 years to degrade when reached the land which causes a great impact on the environment. Moreover, the superabsorbent polymer granules in the absorbent core layer of napkin/diaper may migrate during the usage because of poor integrity between wood pulp and SAP. This migrated SAP may cause discomfort to the wearer.

In this research, a bio-degradable superabsorbent fiber was developed using a cellulose derivative and bio synthetic polymer namely Hydroxyethyl Cellulose (HEC), Poly Vinyl

Alcohol (PVA) and Citric Acid (CA). Electrospinning technique is used to produce the superabsorbent fibrous web/mat for high absorption application. The developed electrospun web was characterized by SEM, FTIR.

Further, the effect of various concentrations (0%, 2%, 4% and 6%) of CA on free absorption capacity (FAC) and absorption under load (AUL) of test samples were studied in distilled water and synthetic blood. The results showed that the electrospun superabsorbent fibrous web namely HEC/PVA/CA4% higher FAC% and AUL (g/g) than all other samples. This structural form of fibrous web could be used as potential superabsorbent for hygiene application.

10.3 Analytical Expression for Steady State Non-Linear Reaction Diffusion Equation in the Electroactive Polymer Film Homotopy Analysis Method

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In this article, we propose a simple and effective method to resolve the steady state non-linear equation that occurs in the context of the electroactive polymer film. According to this mathematical model, a substrate and an immobilized catalyst form a complex. By applying Homotopy Analysis Method, an approximate analytical expression of concentration of substrate for planar electrode is obtained. This obtained analytical solution is compared with numerical results and discovered to be in good agreement. The Homotopy Analysis Method(HAM) generates an efficient sequence of analytical approximations for parametric simulations that are quickly convergent, conveniently computed and easily verifiable.

10.4 Molecularly imprinted polymers for Metal sensing.

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Metal plating, paints, and battery industries accidentally release hazardous metal ions into the environment. It is crucial to monitor or remove these hazardous substances from the environment. MIPs, or molecularly imprinted polymers, can monitor these harmful metals with high selectivity. The foundation of this technology is the "lock and key" concept, which was first used for enzyme-substrate recognition. Due to "functional group template" and "functional group monomer" interactions, a class of polymerisation procedures can be employed to create a MIP that is started by the self-assembled functional monomers around the molecules of templates. In this work, a cadmium ion-imprinted polymer (MIP) was Analysis surface imprinting, using aniline, dimethoxy aniline and sulphanilic acid as a functional monomer and crosslinker. The MIP was characterised by transmission electron microscopy, infrared spectroscopy, and thermal gravimetric analysis. The maximum adsorption capacities of the MIP and non-imprinted polymer for Cadmium ions respectively. The advantage of this technology is that the adsorption removes metal and dye effluents from the sample, and the desorption makes the binding sites reusable for the next cycle. MIPs are a kind of polymers formed by the size, shape and specific functional groups of the template molecule. It is a technology, with its significant adsorption capacities and reusability, that can be resourcefully used for toxicity removal progressions on the industrial level for making a healthy and hearty environment

Keywords: Electrochemical sensor, Molecular imprinted polymer, cadmium.

10.5 Polyvinyl alcohol assisted preparation of silk fibroin and sodium alginate composite film incorporated gold nanoparticles for antibacterial activity

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It is important to improve the antibacterial properties and maintain the desirable humidity of wound dressings. Herein, novel antibacterial wound dressings were prepared. In this present work, polyvinyl alcohol-assisted silk fibroin and sodium alginate are combined with gold nanoparticle hybrids in the composite film developed by the solution casting method.

The casting method is most suitable for the film preparation process. The polyvinyl alcohol, silk fibroin, sodium alginate, and gold nanoparticle hybrid of the composite film are one of the best biomaterials for biomedical applications. The silk fibroin (SF) and sodium alginate (SA) gold nanoparticles (AuNPs) hybrid composite film have antibacterial activity against various pathogenic microorganisms. The preparation of PVA/SF/SA and PVA/SF/SA/Au composite films and their analysis by different characterization methods such as FTIR, SEM, UV-DRS, TGA, and mechanical properties. These are systematically analysis in antibacterial activity study. The coated composite films show the excellent antibacterial activity against gram-positive and gram-negative bacteria. Thus, the obtained properties of composite films reveal the potential of this material, which can be used as an bacterial pathogens.

Keywords: silk fibroin, sodium alginate, gold nanoparticles, antibacterial activity.

10.6 IR responsive liquid crystal elastomer composite films containing conjugated polymer

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Liquid crystal elastomer (LCE) is one such soft actuator which exhibits a spontaneous reversible deformation in response to external stimuli [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, conjugated polymers etc. Conjugated polymers are efficient infrared (IR) light absorbers and when used dopant in LCEs, IR actuating LCE composite can be obtained. In this regard, we have prepared LCE-polyaniline composite films and their response to IR radiation is investigated. The elastomers and composite films are prepared following Finkelmann's hydrosilylation method [2]. Polyaniline is prepared through oxidative polymerization method [3]. Different wt% of polyaniline are incorporated into LCE during the preparation to obtain the composite films. The films are characterized using FTIR, UV-DRS, SEM, and Tensile tests. The thermal and IR actuation of the films are studied and the results are presented.

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

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10.7 Strontium loaded Polylactic Acid (PLA)/Cellulose Biodegradable Membrane for Guided Bone Regeneration.

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Polylactic acid is a polyester polymer that is recyclable and renewable as well. Membrane made of polylactic acid (PLA) is gaining attention nowadays due to its superior properties and versatility in applications. The novel Strontium (Sr2+) loaded Polylactic Acid (PLA)/Cellulose membrane is developed in this study. Sr2+ has the ability to influence osteoblasts, resulting in increased bone formation capacity. (Sr2+-(PLA)/cellulose) asymmetric membranes were synthesised by phase separation and proposed for use in Guided Bone Regeneration. The produced membrane with an asymmetric porous structure possesses hydrophilicity, which is characterized by scanning electron microscopy (SEM), X-ray diffraction spectroscopy (XRD), and thermogravimetric analysis (TGA). The novel materials were investigated with regard to their potential as supports for cell growth in bone repair using multipotent mesenchymal stromal cells (MSC) as a model. MSC are multipotent cells differentiating into osteoblasts, adipocytes, or chondrocytes become a source of cell-based therapy. In biological in-vitro experiments, (Sr2+-(PLA)/cellulose) membrane is favour for osteogenic and antibacterial properties, which have high potential for application in the Guided Bone Regeneration procedure.

Keywords: Polylactic acid; Cellulose; Strontium: Membrane; Guided bone regeneration

10.8 Investigation of protein-based biopolymers with noble metal nanoparticles hybrid of the composite nanofiber for wound healing activity of sparge-dawley rat animal

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A newly designed bimetal blended of palladium and platinum nanoparticles combined with silk fibroin and collagen composite nanofiber was prepared through the electrospun method. The silk fibroin and collagen composite matrix are combined with palladium and platinum nanoparticle are highly enhance the therapeutic agent and more significant for used in wound dressing applications, because these nanofiber scaffolds can easily stimulate the cellular response activity for wound healing sites. Additionally, silk fibroin and collagen matrix are the most abundant amino acids, hence easily reducing and stabilizing agents for metal nanoparticles. The physiochemical, morphological, and thermal properties of composite nanofibrous scaffolds have been interpreted using various characterization techniques such as ATR-FTIR, FE-SEM with EDX, TEM, AFM, XPS, and TGA. The fabrication of SF/CL and SF/CL/Pd-Pt composite nanofiber mats was analyzed by invivo studies for wound healing activity in male Sparge-Dawley rat animals. The wound healing activity treated by the composite nanofiber served as the positive control, and medical gauze served as the negative control. Moreover, the SF/CL/Pd-Pt composite nanofiber had the fastest reepithelization, granulation, and superior angiogenesis properties for enhanced tissue regeneration. These findings demonstrate that the SF/CL/Pd-Pt composite nanofibrous scaffolds were excellent wound dressing materials.

Keywords: Electrospun; nanofiber; silk fibroin; collagen; wound dressing; tissue engineering.

10.9 Synthesis and characterization of azo-containing diacrylate-terminated liquid crystal monomer

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Liquid crystal elastomers (LCEs) are fascinating materials having potential applications in a variety of fields such as sensors, actuators, and soft robotics[1]. LCE can be prepared using different methods such as radical polymerization, hydrosilylation and click reaction.Recently, the click reaction has gained considerable interest over the other methods due to several advantages such as ease of the reaction, feasibility, high yield etc. Diacrylate-terminated compounds are important components of the click reaction to prepare the main-chain liquid crystal elastomers [2]. Further, acrylate compounds are known to react better than the ene/amine/epoxy compounds in the thiol-Micheal addition click reaction.In this present work, synthesis of an azo-containing diacrylated monomer is described. The monomer is synthesized starting from 4, 4′-dihydroxyazobenzene. The synthesized compound is well characterized using IRand NMR. The photophysical properties of the compound are studied using UV-vis spectroscopy. Further, the mesophase behaviour of the compound is investigated under polarized optical microscopy. The compound displayed a smectic phase. This monomer can be effectively employed for the preparation of elastomers through the thiol-acrylate click method and as a cross-linker in radical polymerization and hydrosilylation reactions.

Keywords: Liquid crystal elastomer, Acrylate monomer, Azobenzene

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11.Subramolecular Chemistry

11.1 Synthesis and characterization of trans cinnamic acid methyl ester derivatives and their inclusion complexes studies with cyclodextrins and biological applications

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The main objective of the abstract is to synthesize different trans-cinnamic acid methyl ester derivatives. Further, these compound inclusion with cyclodextrins. The stoichiometric ratio determined by the Benasi-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, 1HNMR XRD, DSC, and SEM. Antifungal and antibiofilm studies performed in the inclusion complex system exhibit a superior antifungal activity compared to the synthesized molecules.

Keywords: cinnamic acid, α- and β-Cyclodextrin, fluorescence, antifungal activity.

11.2 Synthesis and characterization of ethyl cinnamate, formation of an inclusion complex with γ-cyclodextrin, and investigation of its antibacterial activity

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The cinnamic acid derivatives of Ethyl Cinnamate (EC) were synthesized. And their product is elucidated by 1H-NMR and FT-IR Spectroscopy. The confirmed EC and γ-Cyclodextrin inclusion complex formation are studied by UV-Visible and fluorescence spectroscopy. The cyclic voltammetric techniques were used to analyze the formations of the inclusion complex. The stoichiometric ratio of the inclusion complex (1:1) was calculated by Job's plot and binding constant (K) through the Benesi-Hildebrand plot. Thermodynamic parameters (ΔG) were calculated using the Gibbs-Helmholtz free energy equation. This suggests that this inclusion complex formation was spontaneous. The molecular interaction of EC with the hydrophobic cavity of γ-CD was characterized by 2D-1H-NMR(ROESY). The inclusion complex exhibits remarkable antibacterial activity.

Keywords: Cinnamic acid, Ethyl Cinnamate, γ-Cyclodextrin, Inclusion complex.

11.3 Preparation of Gallic acid Functionalized Silver nanoparticle supporting with PVA/β-CD polymeric antimicrobial films for food preservative applications

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Gallic acid (GA) and silver nanoparticles (Ag-NPs) are coupled with polyvinyl alcohol/β-Cyclodextrin (PVA/β-CD) to create PEG plasticized PVA-β-CD@AgNPs/GA film was prepared by casting method, simultaneously this material used for the PVA and PVA-β-CD@AgNPs films for comparison studies. These findings demonstrated that the addition of GA increased film thickness while substantially reducing moisture content and swelling characteristics. The Ag-NPs particle size and function group have been investigated using the UV, FT-IR, and TEM techniques. Using SEM, XRD, XPS, and TGA, the morphological, structural, mechanical, and thermal properties of films were identified. Calculating the amount of Ag ions emitted from the films in an aqueous solution required UV-Vis Spectroscopy. DPPH radical test was used to measure the antioxidant activity. Escherichia coli was the target bacterium, while Aspergillus niger was the target fungus in the antimicrobial activity study. Due to their extraordinarily large surface area, and antibacterial, and antioxidant properties, the multifunctional films made from GA and Ag-NP may be highly useful in food packaging. These components could be used to package fruit and juice that has been preserved.

Keywords: PVA-β-CD@AgNPs/GA, antimicrobial, DPPH radical, Food packaging

11. 4 synthesis and characterization of ethyl (e)-6-methyl-2-oxo-4-styryl-1,2,3,4-tetrahydropyrimidine-5-carboxylate and the inclusion complex with β-cyclodextrin, palladium modified β-cyclodextrin for sensing and microbial applications

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The ethyl (E)-6-methyl-2-oxo-4-styryl-1,2,3,4-tetrahydropyrimidine-5-carboxylate (EMOSTPC) have successfully synthesized from cinnamaldehyde via the synthetic root of Biginelli reaction. The synthesized compound through FT-IR and 1H-NMR spectroscopic techniques proved the formation. The simple one-step method has to prepare the β-cyclodextrin capped Pd particle. The palladium-modified β-CD further characterized by XRD, EDX, SEM, and TGA. Synthesized EMOSTPC encapsulated within the hydrophobic cavity of β-CD and Pd-β-CD, which stimulate solubility and complex formation. The complex formation was examined by spectrophotometric techniques and calculated binding constant (K) and free energy change (ΔG). In recent years, metal sensing playing a role in the research field. We have analysed the synthesized molecule in metal sensing applications through spectrophotometric techniques. The biological investigation of the EMOSTPC compound and complex with β-CD and palladium-modified β-CD is done successfully here in this part.

Keywords: Synthesis, spectroscopic studies, β-cyclodextrin, complex formation, binding constant, metal sensing

12. Textile Chemistry

12.1 A Novel Study on extraction of Dye from Bougainvillea Bracts its Dyeing Properties on Cotton and Pet: Cotton Fabrics

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The present work carried out on dyeing with natural dye Bouganvillae Bracts it belongs to family Nycetaginaceae.The dye extract has good dyeing property with 100/ cotton fabric and 80.20 PET: Cotton. where both the fabrics were bleached and dyed with mordarns. Dyeing was carried out by Pre mordanting and Post mordanting methods and simultaneously without mordants carried out for reference. The dyed Samples have shown good washing, light and rubbing properties. The dye uptake was measured using computer color matching software. Surface topographic studies (SEM).were done for both the fabrics to view the diffusion of dye molecule inside the pores of the fabrics. dyeing was carried out by 1:20 MLR with 2% dyeing.

KEYWORDS - Bracts, SEM, Topographic, diffusion, MLR-material to liquor ratio.

12.2 Electrochemical Decolourisation of Dye Effluents using catalytic anodes

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Growing global population, climate change, and deteriorating water resources and infrastructure have all urged a need for better water treatment methods. The wastewater generated from dye industrial complexes is treated at the wastewater treatment plants and discharged to the rivers. At this time, many trace harmful organic substances, which are not well decomposed by anaerobic treatment and biological treatment, are discharged together. Most of these residual harmful substances are classified as carcinogens or endocrine disruptors, and they have harmful effects on the environment. On the other hand, the electrochemical oxidation process, which has been continuously attracted attention in recent decades, has a relatively simple system configuration (anodes and

cathodes, electrolytes, power supplies, etc.) and produces oxidants in the electrolysis itself without the addition of artificial oxidants There is an advantage that it can be. In addition, unlike previous high-level oxidation processes, small-scale sites are required and can be easily applied to narrow sites. Electrochemical treatment of dye effluent is a promising technique for decentralized wastewater treatment, owing to its modular design, high efficiency, and ease of automation and transportation. The electrochemical methods for dye effluent treatment technique coupled with solar cells can produce in-site oxidative species that can oxidise dye molecules in a short time and low cost. A two-electrode-based electrochemical reactor was built for this purpose. This device is made up of a titanium mesh that has been MMO (Mixed Metal Oxide) coated and a titanium plate that serves as the cathode. The entire electrochemical setup is housed in a PVC (Poly Vinyl Chloride) pipe. The pipe is vertically mounted and contains an input where dye water enters the system and an outlet where the water is discharged after being electrochemically discoloured. While compared with other methods of decolourisation, like chemical methods, it is cost-efficient and convenient for dye decolourisation. It’s also less toxic and more efficient.

Keywords: Electrochemical decolourisation device, MMO coated titanium mesh, Poly Vinyl Chloride,

12.3 Catalytic degradation of the textile dyes under sunlight using NiO Nanoparticles

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We have reported the eco-friendly green synthesis of NiO nanoparticles using aqueous leaves extract of Wrightia tinctoria (Roxb.). The phytoconstituents in the plant extract act as a reducing agent and stability agent for the nanoparticles formation. The prepared NiO NPs (WT NiO NPs) were characterized by UV-Visible spectroscopy, DRS-UV, FT-IR, Powder XRD and FE-SEM. FT-IR result confirms the reduction and capping potential of the plant extract. The average crystallite size was found to be 26.7nm, which was further supported by FE-SEM analysis. The band gap was found to be 2.88eV. The photocatalytic efficiency of the WT

NiO NPs was determined by degrading the textile dyes like Methyl orange (MO) and Rhodamine B (Rh-B) using H2O2 as an oxidizing agent under sunlight. The rate of the reaction was calculated. The reaction follows the pseudo-first-order kinetics. The results revealed that the WT NiO NPs can be a better photocatalyst for the degradation of textile dyes.

Keywords:Wrightia tinctoria (Roxb.), green synthesis, NiO NPs, photocatalyst, Methyl Orange, Rhodamine B.

12. 4 Interaction of Martius Yellow dye with anionic, cationic and nonionic surfactant mediums

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Dye -surfactant interactions are useful in many application of the dye industry. It helps to identify the most suitable medium in which the dye shows its maximum efficacy. Martius yellow (MY) is a direct dye which is used extensively in staining and dyeing of cotton/rayon. In this work we have explored the interaction of MY in three different surfactant mediums, viz., anionic, sodium dodecylsulphate (SDS), cationic, cetyltrimethylammonium bromide (CTAB), and nonionic, tween 20. The investigations were done through the UV-visible spectroscopy and conductivity measurments. The UV – visible spectra of MY in aqueous solution displayed two major peaks at 429 and 392 nm which is in good agreement with literature. On adding the surfactants there was first lowering of absorbance and on increase of concentration of surfactants the absorbance increased gradually. This symbolizes for active interactions taking place between MY and the surfactants. The thermodynamic parameters determined from conductivity values shows that Gibb’s free energy of micellization, ΔG0m is negative, indicating spontaneous reaction all the three dye – surfactant combinations. This is probably the first report of MY dye in three micellar mediums.

13 Miscellaneous

13. 1 Level of Trace Metal Accumulation and Human Health Risk Assessment of Selected Red and Green Seaweeds Along Thondi Coast, Palk Bay, India

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Using inductively coupled plasma mass spectrometry (ICP-MS), the bioaccumulation of trace metals in 10 different edible red (Gracilaria Salicornia, Gracilaria folifera, Gracilaria eucheumoides, Hypnea valentiae, Acanthophora specifera and Jania rubens) and green (Chaetomorpha crassa, Chaetomorpha indica, Cladophora vagabunda and Valoniopsis panchynema) seaweeds was investigated. Totally 15 elements such as Al, As, Cd, Co, Cu, Cr, Fe, K, Mg, Mn, Ni, Pb, Sr, V and Zn were presented. Iron bioaccumulation in rhodophyta was considerable (8.51 ± 0.19 µg/g), whereas magnesium and strontium levels were lower in the studied seaweeds (0.13 ± 0.02 µg/g and 0.21 ± 0.01 µg/g, respectively). Chlorophyta showed greater levels of bioaccumulation for manganese (4.94 ± 0.15 µg/g), aluminium (4.21 ± 0.18 µg/g), and vanadium (0.09 ± 0.02 µg/g), whereas arsenic (0.18 ± 0.02 µg/g) were at lower levels. The Bio Accumulation Factor (BAF) is an important metric for assessing seaweed's ability to gather metals from the surface water. The Metal Pollution Index (MPI) was developed to determine the extent of trace metal pollution in each macroalgae. The Target Hazard Quotient (THQ) was more than one in all selected green and red seaweed for women, men, and children, implying some degree of health risk in exposed persons. In order to comprehend the consequences of consuming seaweeds by humans, health evaluation studies of seaweed were also done. The results suggest that, in the general population, ingesting macroalgae has no health risks. Additionally, it is important to continuously check the confirmative toxicity of certain metals found in macroalgae, such as Cd, Pb, and Zn. The amount of toxic metals accumulating in the edible macroalgae under investigation is negligible when compared to the maximum level suggested for human consumption by national and international regulatory agencies.

Keywords: Human consumption risk, ICP-MS, macroalgae, metal pollution, Trace metals, seawater

13.2 Assessment of the Physicochemical Parameters of the Coastal Water and Heavy Metal Concentration of the Selected Edible Fishes along Thondi Coast, Palkbay, India

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Heavy metal possesses a great threat to public health because of their high toxicity, abundance and accumulation by various organisms. The present study was conducted to determine physicochemical properties and heavy metal levels in the muscle tissues of five edible fish species- Leiognathus equulus, Lates calcarifer, Sillago sihama, Scolopsis bimaculatus, Lutjanus fulviflamma along the coastal area of Thondi, Tamil Nadu. The objective of the study is to determine the appropriateness of these five fish for human consumption. Data were collected from the month of January 2022 to April 2022. The physicochemical properties of water such as temperature, pH, Salinity, electrical conductivity, TSS, TDS, dissolved oxygen, alkalinity, calcium & magnesium, inorganic phosphate, total phosphorus, nitrate, nitrite and silicate were determined. Atomic absorption spectrophotometry (AAS) was used for the determination of heavy metals such as Copper (Cu), Arsenic (As), Chromium (Cr), Lead (Pb), Cadmium (Cd) and Zinc (Zn) in the muscle tissue of the fishes. Copper, arsenic and lead were found to be highest in Sillago sihama; 1.6102, 1.2364 & 1.0103µg/g respectively, whereas copper was found lowest in Scolopsis bimaculatus; 1.0013µg/g and arsenic & lead found minimum in Lates calcarifer; 0.6216 & 0.8645µg/g respectively. Chromium was found maximum in Lates calcarifer; 1.6781µg/g and minimum in Sillago sihama; 0.9674µg/g. Cadmium and zinc were found maximum in Scolopsis bimaculatus; 0.0876 & 1.0564µg/g respectively and minimum in Lutjanus fulviflamma; 0.0641µg/g and Lates calcarifer; 0.7745µg/g respectively. Health risk assessment was calculated for carcinogenic and non-carcinogenic exposure and the target hazard quotient (THQ) values for all the metals except for As were found to be lower than 1, implying that there might be an adverse health issue due to excessive consumption of these species.

Keywords: Bioaccumulation, Heavy Metal, Health Risk Assessment, Pollution.

13.3 Mathematical modelling and Analytical technique for convection – diffusion equation in Rotating Disk Electrode

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This paper analyses a mathematical model for a rotating disc electrode's convection–diffusion process (RDE). The convection – Diffusion equation is a partial differential equation. Mass diffusion is reported in the study of redox chemical reactions using a simple electron transport process. An approximate analytical solution for the surface contraction and, in application limiting current is calculated using the Homotopy Perturbation method.

Keywords: Rotating Disc Element (RDE), Non-linear differential equation, convection-diffusion equation, Homotopy Perturbation method (HPM)

13.4 Amino acid functionalized drug loaded natural source derived nanohydroxyapatite for orthopedic applications

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Hydroxyapatite (HAp) is one of the naturally occurring mineral form of calcium apatite which is a widely used bioceramic material for various biomedical applications such as tissue engineering scaffolds, coating on metallic implants and carriers for drugs, proteins and biomolecules delivery. Hydroxyapatite is similar to human bone and teeth minerals in structure and composition and also have the properties of good biocompatibility, osteoconductivity, osteoinductivity and bioactivity. Recently, eggshell derived nHAp is gaining much attention for bone regeneration application. In addition, amino acids play an important role in bone mineralization process which regulates the orientation, growth and morphology of hydroxyapatite nanocrystals. Synthesis and characterization of tyrosine functionalized eggshell derived nHAp loaded with doxycycline by wet precipitation method and screening of antibacterial activity against S.aureus will be discussed.

Keywords: Hydroxyapatite, amino acid, S.aureus, Doxycycline, eggshell.

13.5 Effect of Novel Therapeutic medicine Swertiamarin from Enicostema axillare in zebrafish infected with Salmonella typhi

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Herbal treatments have been practiced by humans over centuries and therefore possess time-proven safety. However, it is crucial to evaluate the toxic effects of herbal medicine to confirm their safety, particularly when developing therapeutic drugs. Use of laboratory animals such as mice, rat and rabbits was considered as gold standard in herbal toxicity assessments. However, in the last few decades, the ethical consideration of using higher vertebrates for toxicity testing has become more controversial. As a possible alternative model involving lower vertebrates such as zebrafish were introduced. Hence in the present study, swertiamain compound isolated from E. axillare was assessed for it antimicrobial activity in zebrafish larvae againt S. typhi. The cumulative mortality rate and bacterial localization in zebrafish larvae were studied. Biochemical markers assays were performed to find the preventive role of the compound during the typhoid infection. The results showed that zebrafish can be successfully used as a model to study typhoid infection and the anti-bacterial compound swertiamarin used in this study clears the bacterial load and pathogenic symptoms to a great extent.

Keywords: Typhoid infection, Biochemical markers assays, anti-bacterial compound, Zebrafish Swertiamarin, preventive assay.

13.6 Studies on the Ni-W-Si_3n_4 Nano Composite Coating Prepared By Electodeposition Method

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Ni-W-Si3N4 nanocomposite coating was successfully synthesized on mild steel substrate using direct current and pulse current electrodeposition process in a nickel acetate bath. Ni-W-Si3N4 composite coatings were characterized by X-ray diffraction analysis, Scanning electron microscopy, Atomic force microscopy and Microhardness. Tafel polarization and electrochemical impedance spectroscopy methods were applied to measure the corrosion resistance properties of the nanocomposite coatings in 3.5% NaCl solution. The crystalline structure was face centered cubic (fcc) for electrodeposited Ni-W and Ni-W incorporated silicon nitride. Ni-W-Si3N4 nanocomposite coatings have exhibited significantly improved micro hardness compared to pure nickel coatings due to combination of dispersion strengthening and matrix grain refining. Ni-W-Si3N4 nanocomposite coating resulted in comparatively smooth surface, less friction coefficient, excellent water repellency and superior corrosion resistance. The pulse current nanocomposite coatings have higher micro hardness and excellent corrosion resistance properties than the direct current composite coatings.

Key words: Electrodeposition, Microhardness, Nanocomposite coating, Corrosion study.

13.7 Investigation of Corrosion Resistance of Electrodeposited Ni–Al-Tio_2 Composite Coatings

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Electrodeposition is a most uncomplicated method to generate metal and alloy matrix composite coatings. Ni is particularly interesting because Al-Ni exhibits excellent corrosion resistance and high temperature oxidation resistance compare to various alloy coating. In this way electrodepositions of Ni-Al and Ni-Al-TiO2 nanocomposites coated by direct current and pulse current techniques. The optimize composition of the electrodeposited Ni-Al and Ni-Al-TiO2 nanocomposite coatings were studied by X-ray diffraction analysis and scanning electron microscopy with EDAX and atomic force microscopy and microhardness. Surface morphology studies revealed that Ni-Al alloy surface was covered by long needle like crystals and Ni-Al-TiO2 composite coatings with smaller spherical sized grains. Measurements of microhardness studies revealed that the incorporation of aluminium particles lowers the microhardness of Ni coating due to the high ductility of aluminium and weak bonds between aluminium and nickel. Polarization curves shifted to negative potentials and corrosion rate is decreased incorporation of titanium dioxide particles in Ni-Al matrix.

KEY WORDS: Electrodeposition, TiO2, SEM, XRD, Tafel polarisation

13.8 Facile Synthesis of Nickel Ferrite Nanoparticle; A Voltammetric Food Analytical Sensor for the Determination Of Vanillin

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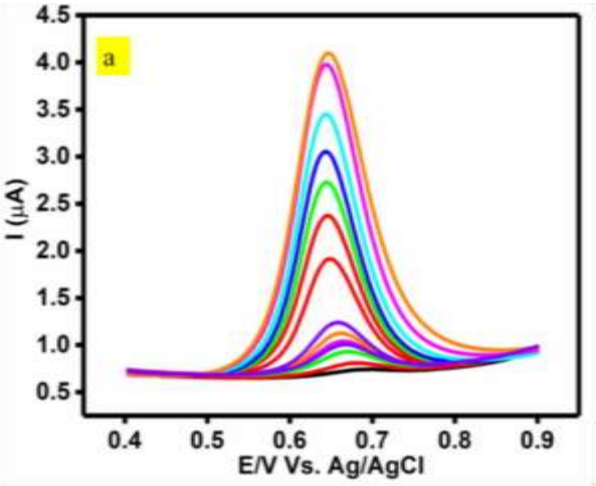
In this investigation, a highly sensitive food analytical sensor was suggested for the determination of Vanillin. The food electrochemical sensor was amplified by NiFe2O3 nanoparticle. The Synthesized NiFe2O3 nanoparticle was analysed through various techniques. Due to the higher surface area, higher stability, improved electrocatalytic activity towards the detection of Vanillin with a low detection limit 0.085 µM and higher sensitivity 36.66 µA µM-1 cm-2 were achieved. The results confirmed that NiFe2O3 is a suitable, stable and fast response sensor for the determination of vanillin. The fabricated sensor can be applicable for the detection of vanillin in a biological use in future.



Keywords: Nickel Ferrite Nanoparticle, Analytical sensor, Vanillin.

13.9 LLDPE resin for Green house film applications using different PAR additives

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This study defines the use of Linear-low-density-polyethylene- (LLDPE with 1 MI & 0.920 density) based formulations with Antioxidants (AO), UV additives and different PAR (Photosynthetically Active Radiation) reflective pigments for the use of Greenhouse film application. The resin products were prepared by melt blending technique using LLDPE pellets, AO additives, UV additives, and PAR pigments. The additives used are for Primary AO (Phenolic group), Secondary AO (Phosphite Group), UV Additives (HALS Group), and different PAR Pigments (TiO2 coated with Mica, Rhodamine – B, Congo Red, Metal Organic group, European Organic Chemical). The study comprised of these different PAR pigments for the enhancement of Greenhouse films and the growth of the plants.Initially, the extruded resin samples and their subsequent films were prepared by blown film extrusion process have been analyzed for different analytical parameters.The pellets were analyzed for Melt flow properties, Density, Thermal properties, Rheology properties were analyzed. The film samples were analyzed for Optical properties, Mechanical Properties, UV light transmittance. The results showed that the melting and crystallization temperatures (Tm and Tc, resp.) of these formulations were almost similar to that of control resin. The melt

viscosity was measured by stress-controlled rotational rheometer and melt flow index (MFI) instruments. Rheological measurements indicated that the blend formulations with NIR-reflective additive have similar melt viscoelastic behavior (storage modulus and dynamic viscosity) to the control resin. The mechanical test performed on NIR-reflective films showed similar values of tensile strength for blend samples as that of control resin. The spectral radiometric properties of the blend films were evaluated in the solar wavelength range of 200–1100nm and found to be improved over the control sample with PAR-reflective pigment in the wavelength range of 400-700nm.

13.10 A facile strategy to preparation of ZnO, Cu^{2+} - ZnO and Co^{2+} - ZnO nanoparticles with superior catalytic reductive degradation behavior under methylene blue via wet-chemical process

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Present work, green approach of ZnO, Cu2+ - ZnO and Co2+ - ZnO nanoparticles were synthesized using STL extract as reducing as well as stabilizing agents. The obtained samples were characterized using different approaches as XRD, FT-IR, SEM-EDX, UV-visible and BET measurements were used for the structural, morphological, and optical properties in nanoscale region. The cubic phase with the particle size were observed as 30-40, 22-30 and 10-20 nm, respectively by XRD and SEM analysis. In addition, the percentage degradation were found to be 63.5 %, 82.5 %, and 93.8 %, within 120 min of UV light irradiation using MeB in the presence of ZnO, Cu2+ - ZnO and Co2+ - ZnO respectively. Moreover, the pseudo-first order reaction rate constants were found to be 0.00298 min-1, 0.00345 min-1 and 0.00365 min-1 respectively. Among catalyst results, Co2+ - ZnO particles enhanced highest capability to photo- degrade the pollutants as MeB due to the generation of heterojunction interface among individual constituents. Consequently, it can be anticipated that Co2+ - ZnO particles could be used as multifunctional photocatalyst for the treatment of different environmental pollutants.

Keywords: ZnO; Cu2+ - ZnO; Co2+ - ZnO NPs; STL extract; Optical; Catalytic.

13. 11 Electrochemical investigation of the influence of different plasticizers in poly(vinylidene-co-acrylonitrile) based gel polymer electrolytes

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The development of electronic gadgets necessitates for high energy density batteries. In recent years, large scientific and technical interest in lithium polymer secondary batteries leads to the development of electrolytes with high electrochemical windows. Several researches deliberate the performance of polymer electrolytes owing to its high energy density, ease of preparation, compatibility between the electrodes etc. Numerous strategies are followed to match the ionic conductivity and mechanical stability of polymer electrolytes. This work describes the clear effect of plasticizer on the performance of lithium ion batteries with four different plasticizer such as ethylene carbonate (EC), propylene carbonate (PC), γ-Butyrolactone (γBL) and diethyl carbonate (DEC) were used. Gel polymer electrolytes comprising of PVdC- AN (52wt%) – $LiClO_4$ (8wt.%)–ZrO_2 (6wt%)- X(40) (X- EC,PC, γBL, DEC) were prepared by solution casting technique. The structural and complexation formation of the prepared electrolytes have been confirmed by XRD and FTIR analysis. The effect of plasticizer on ionic conductivity is depicted using a.c impedance studies in the temperature range 303 -363 K. The highest ionic conductivity value 1.2×10^{-3} S/ cm was measured for the sample incorporating EC, owing to its high dielectric constant (89.6). Thermal stability of the samples has been examined using TG/DTA. The maximum conducting sample, with plasticizer EC can be operated up to 160 °C. The morphology is analyzed by SEM.

13.12 Electrospun based polyvinyl alcohol assisted silk fibroin and sodium alginate composite nanofibers incorporated silver nanoparticles for Antibacterial activity

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The electrospinning method is a low-cost process for the preparation of nanofiber matrix. In recent years, its application to the development of multifunctional materials has encountered biomedical applications. In this paper, we briefly overview the general aspects of electrospinning and then focus on the organic and inorganic materials used in the fabrication of composite nanofiber scaffolds. This research focuses on the electrospun-based fabrication of composite nanofibers using polyvinyl alcohol-assisted ternary composites. The ternary composite of silk fibroin, sodium alginate, and silver nanoparticle hybrid of the composite nanofiber is one of the most effective biomaterials for enhancing biomedical applications. Nowadays, nanofiber material is most advantageous for biological activity because of its unique properties, such as high biocompatibility and biodegradability. Silk fibroin (SF) is prepared from Bombyxmori silkworm cocoon. Sodium alginate (SA) is a natural hydrophilic polysaccharide derived from marine brown algae. The silver nanoparticle (Ag) is most beneficial for antimicrobial activity. The fabrication of PVA/SF/SA, and PVA/SF/SA/Ag composite nanofiber analysis of different characterization techniques, such as Physiochemical study for fourier transform infrared spectroscopy (FTIR) and ultraviolet differential reflectance spectroscopy (UV-DRS), morphological study of composite nanofiber confirmed by field emission scanning electron microscopy (FESEM), thermal stability study for thermogravimetric analysis (TGA), and mechanical strength analysis in composite nanofiber The antibacterial activity of the prepared composite nanofiber analysis were investigated.

Keywords: Electrospun; silk fibroin; sodium alginate; silver nanoparticles; antibacterial activity.

13.13 An Easy Synthetic Approach of Rare ***Earth*** Mixed Transition Metal for the Electrochemical Oxidation of Antipsychotic Drug

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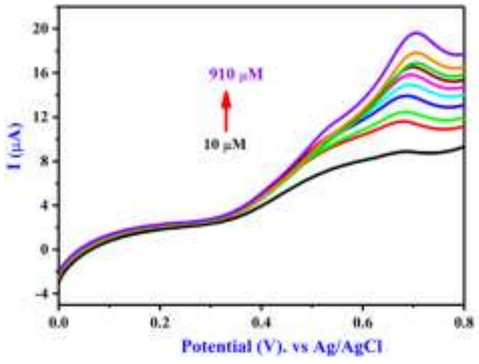
For the first time, we are successful in the synthesis of structurally specific LaVO4 nanoparticle using hydrothermal followed by calcination method. The LaVO4 nanoparticle formation was conformed using UV, FT-IR, XRD analysis. The electrochemical characteristics were performed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV), and amperometric (i-t) techniques. This nanoparticle has been utilized as an electrode modifier for the electrooxidation of Olanzapine. Furthermore, it has been found to show the enhancement in peak current and shift of the oxidation potential in a negative direction by comparison to bare GCE. Due to the higher surface area, higher stability, improved electrocatalytic activity towards the detection of Olanzapine with a low detection limit 1.145 µM and higher sensitivity 13.33 µA µM-1 cm-2 were achieved. It is expected that LaVO4/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of Olanzapine.



Keywords : LaVO4, Nanoparticle, Electrocatalytic activity, Biosensor, Olanzapine.

13.14 Enhanced Electrochemical Activity of An Antagonist Drug via Facile Synthesis of Strontium Molybdate

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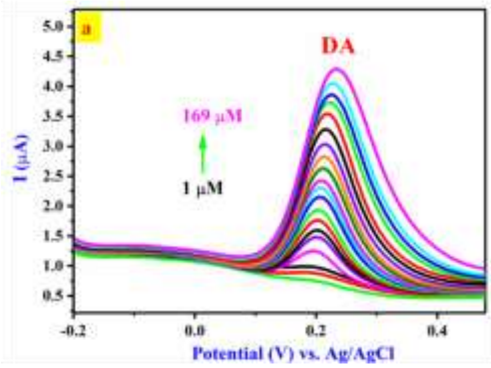
In this study, we developed the synthesis of Strontium Molybdate (SrMoO4) using hydrothermal followed by calcination method. The SrMoO4 nanoparticle formation was conformed using UV, FT-IR, XRD analysis. The electrochemical characteristics were performed by cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), differential pulse voltammetry (DPV), and amperometric (i-t) techniques. This nanoparticle has been utilized as an electrode modifier for the electro oxidation of Dopamine. Furthermore, it has been found to show the enhancement in peak current and shift of the oxidation potential in a negative direction by comparison to bare GCE. Due to the higher surface area, higher stability, improved electro catalytic activity towards the detection of Dopamine with a low detection limit 1.39 µM and higher sensitivity 27.69 µA µM-1 cm-2 were achieved. It is expected that SrMoO4/GCE is a good candidate for low-cost and highly sensitive biosensors for the detection of Dopamine.



Keywords: Strontium Molybdate, Biosensors, Antagonist Drug, Dopamine.

13.15 Cu-Co bimetallic nanocomposits on g-C_3N_4 nanosheets as peroxidase mimic for glucose and ascorbic acid detection

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The catalytic properties of bimetallic nanoparticles (NPs) have been proven in several investigations to be superior to those of their monometallic counterparts. In this research, bimetallic Cu-Co NPs are deposited on nanosheets of g-C 3 N 4 using a wet-chemistry technique. Benefiting from the synergistic interaction between g-C 3 N 4 and metallic NPs, this nanocomposite displays remarkable intrinsic peroxidase-like activity. Peroxidase substrates like 3,3′,5,5′-tetramethylbenzidine (TMB) can be reacted with hydrogen peroxide with the use of this activity as a catalyst. Nanocomposite benefits from both g-C 3 N 4 and metallic NPs (H2O2). Combining the peroxidase-like activity of the Cu-Co/g-C 3 N 4 nanostructures with the activity of glucose oxidase allowed us to build a sensitive and selective colorimetric test for glucose detection in blood serum with a detection limit of 3.8 M. (GluOx). So the assay could be built, that is. The monometallic analogues' detection thresholds were calculated to be 7.9 M (for Co/rGO) and 9.7 M (for Cu/rGO). The Cu-Co/g-C3N4 nanostructures were also effectively used to detect ascorbic acid at a sensitivity of 3.6 M. These nanostructures demonstrated their potential once Coain.

Keywords: g-C3N4 Copper-Cobalt bimetallic nanocomposites, Sensing, Peroxidase, Glucose, Ascorbic acid.

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