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IGMSE - 2023

Engineer to Excel

SIMATS ENGINEERING

INTERNATIONAL CONFERENCE ON

INNOVATIVE GREEN MATERIALS FOR SUSTAINABLE ENGINEERING

(IGMSE-2023)

Organized by

Department of Chemistry

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Dr. N. Srinivasan
Dr. S. Arunachalam
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Co-convenors:
Dr. N. Prakash
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IGAUGE PLATINUM · Internal Quality Assurance Cell · Institution's Innovation Council (Ministry of Education Initiative) · MoE's INNOVATION CELL (GOVERNMENT OF INDIA) · SUSTAINABLE DEVELOPMENT GOALS

International Conference on
Innovative Green Materials for Sustainable Engineering
(IGMSE-2023)

27th & 28th February 2023

Book of Abstracts

Convenors

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Department of Chemistry
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CHANCELLOR'S DESK

It is admirable that SIMATS has developed a progressive system to empower both staff and students to improve their skills and talent in multiple fields including sciences, medicine, and technological disciplines to cope with the progressive changes in the modern day. SIMATS School of Engineering has been on the frontline among academic institutions in providing the best education to students through effective teaching modules and learning environments. SIMATS highly encourages Research & Innovation and supports scientific events which are crucial parts of academics to maintain high standards in education to contribute to a nation's development. It gives me great pleasure to invite delegates to our campus to the International Conference on Innovative Green Materials for Sustainable Engineering (IGMSE-2023), 27th & 28th February 2023.

I take this opportunity to congratulate all the faculty of the Department of Chemistry for their efforts and initiative toward the success of the program.

Dr. N. M. VEERAIYAN

CHANCELLOR, SIMATS

VICE- CHANCELLOR'S DESK

I am extremely happy to know that the Department of Chemistry, SIMATS School of Engineering is organizing a two-day International Conference on Innovative Green Materials for Sustainable Engineering during 27th & 28th February 2023.

I believe that the conference will not only provide a useful forum to the participants to share their expertise for extending collaboration in their fields but will also be professionally beneficial to them. It will also help to familiarize the participants on the advanced research happening around the oarless.

I wish the organizers a great success in their endeavour.

Dr. CHADARAM SIVAJI

VICE CHANCELLOR, SIMATS

DIRECTOR OF ACADEMICS DESK

It gives me immense pleasure and pride to be a part of the International Conference organized by the Department of Chemistry, International Conference on Innovative Green Materials for Sustainable Engineering during 27th & 28th February 2023 in SIMATS School of Engineering.

The motto of the Conference is to bring together experts from academic institutions, industries and researchers for sharing knowledge, expertise and experience in the emerging trends related to sustainable engineering education. I appreciate the efforts undertaken by the SIMATS School of Engineering team in organizing the International Conference to create a platform for experts to share and learn.

I congratulate all the concerned members and wish the conference a grand success.

Dr. DEEPAK NALLASWAMY

DIRECTOR OF ACADEMICS,

SIMATS

DIRECTOR'S DESK

It is a great pleasure and honour for me to invite all the great scientists, academicians, young researchers, delegates, and students to the International Conference on Innovative Green Materials for Sustainable Engineering on 27th & 28th February 2023 being organized by our SIMATS School of Engineering.

I strongly believe that research, innovation, and collaboration are key to success in a sustainable world. At SIMATS School of engineering, we are dynamically engaged in creating a research environment to promote novel research with a strong application focus in multi-disciplinary areas. We are organizing conferences to provide an essential perspective and expertise in continuously emerging trends & practices of science and engineering. In the modern era, the evolution of green materials and applications is vital to tackle the environmental problems due to globalization and population. I strongly believe that the International Conference on ***Innovative Green Materials for Sustainable Engineering*** will offer an excellent opportunity for the delegates to identify the problems and give an insight into the hot research areas and cutting-edge technologies in green materials to catalyse interdisciplinary thinking to solve the issues.

I appreciate the department of Chemistry for its commitment and vision toward research. I hope that the conference enriches all with many modern ideas and innovative thoughts that will be fruitful for the researchers in their future endeavours

I congratulate the team and wish you all the success.

Dr. RAMYA DEEPAK

DIRECTOR,

SIMATS School of Engineering

PRINCIPAL'S DESK

Warm and Happy greeting to all. I am immensely happy that the Department of Chemistry is organizing two days International Conference on International Conference on Innovative Green Materials for Sustainable Engineering during 27th & 28th February 2023.

The theme of the conference about Innovative Green Materials for Sustainable Engineering is very appropriate and I hope that this conference will provide a common platform for the academicians; researchers and industrialists to share their knowledge and experience about recent advancements in Sustainable engineering development.

I appreciate the active interest and participation shown by the faculty members of the Department of Chemistry in organizing International Level conferences, Webinars, Workshops and maintaining the research ambience in the Department.

I wish the department all the very best in all their sustained pursuits for excellence and their earnest efforts in making a conference a grand success.

Dr. B. R AMESH

PRINCIPAL,

SIMATS School of Engineering

DEPARTMENT MESSAGE

The Department of Chemistry strives to produce engineers with a broad understanding of fundamental chemistry so that they can develop, innovate, and contribute to technological growth. The Department of Chemistry, SIMATS School of Engineering is organizing two days International Conference on Innovative Green Materials for Sustainable Engineering (IGMSE-2023) during 27th & 28th February 2023 which aims to bring together leading academic scientists, researchers and research scholars to exchange and share their experiences and research results on all aspects of Science and Technology and Humanities. It also provides a premier interdisciplinary platform for researchers, practitioners and educators to present and discuss the most recent innovations, trends, and concerns as well as practical challenges encountered and solutions adopted in the fields of Science and Technology and Humanities.

We would like to extend our heartfelt thanks and gratitude to Dr. N. M. Veeraiyan, Chancellor-SIMATS, Dr. Chadaram Sivaji, Vice-Chancellor-SIMATS, Dr. Deepak Nallasamy – Director Academics, SIMATS, Mrs. Ramya Deepak, Director, SIMATS School of Engineering and Dr. B. Ramesh, Principal, SIMATS School of Engineering for providing us all the required support in organizing IGMSE-2023. We thank the various Institutions, Industries and Research organizations for deputing delegates to participate in the Conference. We thank all the sponsors for their contribution to this event. We thank the National and International Advisory Committee for their valuable suggestions and the organizing committee members for their contributions to the Conference.

Convenors, Co-Convenors, Organizing Members,

Department of Chemistry,

SIMATS School of Engineering

List of Abstracts

Keynote Speakers ABSTRACTs

Imperative Green Materials for Potential Catalytic Applications: An Overview

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ABSTRACT

It is noteworthy to mention that catalysts are playing a very critical role in accelerating any chemical reactions that are occurring to produce lower chemical yield even at a longer reaction time. Hence, any industries looking for highest product yield obviously should depend on catalyst. It is also necessary to highlight here that certain pharmaceutically connected lifesaving product yield reactions usually performed from immiscible substrates. But it is very difficult to perform immiscible substrate liquid phase reaction even with addition of normal catalyst. Therefore, it is necessary to mention that to perform immiscible substrates reaction one should employ specialized catalyst.

In the current scenario, Phase transfer catalyst (PTC) is an indispensable tool to carry out the novel organic transformation involving reagents soluble in immiscible solvents. The specialty of phase transfer catalyst is to transfer one of the reactants in one phase to the other, where it can rapidly react with another reactant. This technique is simple to carryout, requires mild reaction conditions and can be applied on a commercial scale too. In recent years, the employability of PTC has been drastically increased, owing to its operational simplicity, high reaction rate, high yield and selectivity. The prime merits of insoluble multi-site PTC includes, getting higher yield as compared with single - site PTC and more importantly the recovery of the catalyst is more easy from the reaction mixture and its recyclability is quite possible.

Dendrimers are attractive candidate for catalytic applications and they can act as catalytically active species, as well as, soluble supports. Different types of dendrimer-encapsulated Metal nanoparticles were used as catalytic moiety both in homogeneous and in heterogeneous catalysis. Examples of dendrimeric catalysts include chiral dendrimer catalysts applied in enantioselective catalysis. Chiral dendrimer catalysts with a high level of molecular monodispersity, structural regularity and well-defined catalytic sites can be prepared either by attachment of achiral complexes to chiral dendrimer structures or by immobilization of chiral catalysts to achiral dendrimers.

In view of the significant merits noticed in PTC, insoluble multi – site PTC and soluble/ insoluble dendrimer stabilized nanoparticle catalysts, several pharmaceutically significant immiscible substrate reactions were performed in a simplified experimental route and produced appreciable quantum yield with highest activity and selectivity.

Nanomaterials: Decades of Small Materials Doing Wonderful Things for Humans and the Environment

Thomas J. Webster, Ph.D.

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ABSTRACT

Nanomaterials have been revolutionizing numerous industries for decades. With the announcement of the National Nanotechnology Initiative in the U.S. in 2000 and elsewhere, research in nanomaterials has accelerated as well as commercial products containing nanomaterials. In particular, nanomaterials have improved the sensitivity of sensors. Nanomaterials have reduced the size of electronics. Nanomaterials have also been used as medical devices improving the lives of millions. In particular, one study indicates the implantation of nanotextured spinal implants into over 14,000 patients over the past 5 years with no cases of infections or other implant failures; significantly better than statistics on conventional spinal implants which have up to 20% failure rates. Recently, nanomaterials have even been improving the environment. All of these and other very exciting advancements of nanomaterials will be covered in this talk with an eye on what the future holds for nanomaterials and nanotechnology. One thing is clear over the past several decades, nanomaterials have changed society for the better and will continue to do so in the decades ahead.

Photoelectrochemical Water Splitting: A Journey from Lab Scale to Prototype Device

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ABSTRACT

Extensive use of fossil fuels leads to depletion of its natural resources and increasing the demand of energy thus make the environmental impact. The development of a clean, green and renewable energy carrier that does not utilize fossil fuels is a great scientific and technological challenge. Solar energy has gained tremendous attention with great prospects to settle the worldwide environmental pollution and energy shortage issues. The use of hybrid or composite nanomaterials to harvest solar energy as well as generate the electricity and hydrogen seems to be the most excellent way to meet the near-future energy demand. Photoelectrocatalytic water splitting offers a promising method to harvest the solar energy into renewable hydrogen energy. This talk will discuss about the the advances in the development of efficient photoelectrocatalytic materials. First, the fundamentals involved in the photoelectrocatalytic water splitting will be elaborated. Then, the critical properties of photoelectrocatalytic materials are classified and will discussed according to the associated processes, including light absorption, charge separation, charge transportation, and photoelectrocatalytic reactions. The importance of heterointerfaces in photoelectrodes will be mentioned in conjunction with the illustration of some heterojunction photocatalytic materials. Also, some strategies involved in material screening and optimization for the construction of highly efficient photoelectrochemical devices for water splitting will be discussed. Some background about bismuth based metal oxides and graphitic carbon nitrides including synthesis, properities and performance in water splitting will be discussed.

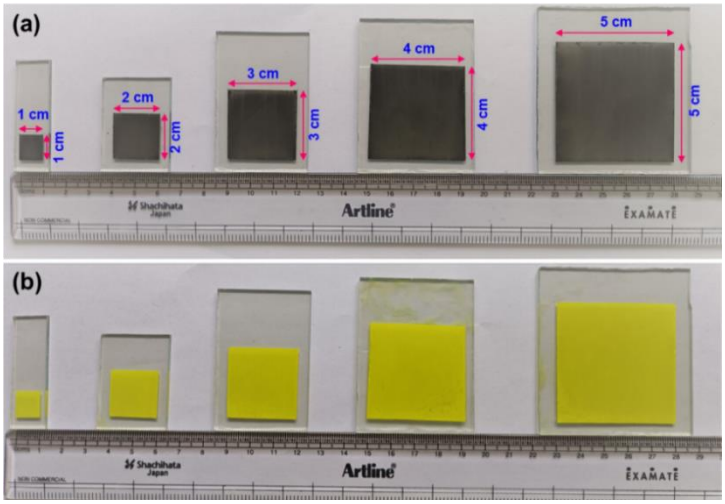

Figure: Photograph images of (a) Bi electrodes *via* electrodeposition and (b) $BiVO_4$ electrode.

Finally this talk further highlights the recent developments with the bismuth and graphitic carbin nitride based heterojunction hybrid materials in these area and indicate some specific examples for improved photoelectrocatalytic water splitting performance. Further, roadmap for the lab scale to prototype also demostrated.

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Chemistry of *N*-nitrosamines: From synthesis to applications

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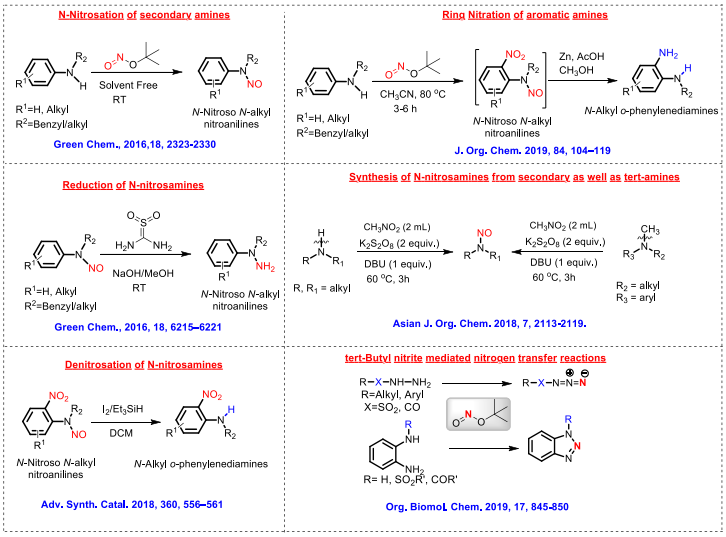
ABSTRACT

N-Nitroso compounds present in a wide range of foods, cosmetics and natural products.[1] More attention is being paid to the chemistry of *N*-nitroso compounds owing to their unique carcinogenic and mutagenic properties.[2] These compounds have been used in various treatments including cancer, cardiovascular diseases, central nervous disorders, and diseases related to immunity and physiological disorders.[1-2] Besides the biological importance, *N*-nitrosamine compounds have become valuable intermediates in organic synthesis.[3]

In this context, our group recently developed an efficient and green method for the preparation of *N*-nitrosamines from corresponding secondary amines under solvent, acid and metal free condition using *tert*-butylnitrite (TBN).[4s] In continuation, we have developed a metal free method for the reduction of *N*-nitrosamines to corresponding hydrazines using green industrial reductant thiourea-dioxide (TDO).[4b] In addition to these transformations, we have also developed an efficient method for the direct nitration of aryl secondary amines through *N*-nitroso intermediates[4c] as well as de-nitrosation of aryl N-nitrosamines.[4d] The presentation will cover our recent achievements in this area of research.



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Advanced Functional Organic and Inorganic Materials: Optoelectronic and Sustainable Catalysis Applications

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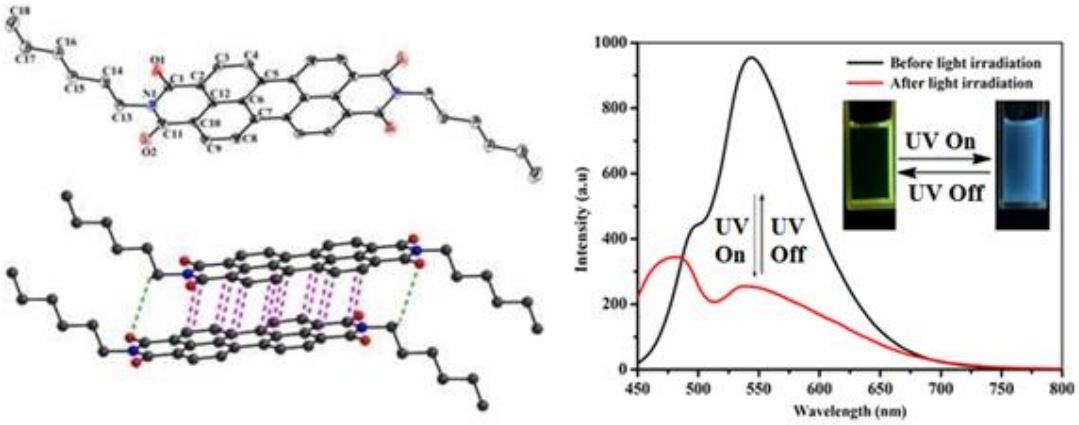
ABSTRACT

Stimuli-responsive smart materials have considerably attracting interest in current research area in order to achieve optoelectronic devices, semi-conductors, sensors, resonant energy transfer and intermolecular charge transfer materials, photovoltaics, photoinduced electron transfer materials, organic light emitting diodes (OLED), organic thin-film transistors (OTFT), photodetectors and so on. In this talk, I would like to present our recent results on organic and inorganic based advanced functional materials for multifunctional applications including thermochromism, solvatochromism, photofluorochromism, mechanofluorochromism and photoswitching. Besides, development of TM-NNN (TM=Ni, Co and Mn) complexes for sustainable catalysis will also be discussed.



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The Role of Various Supports in Metal Nanoparticles Catalysts

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ABSTRACT

A supported metal nanoparticles (NPs) catalyst plays a vital role in bulk synthesis of important raw chemicals, renewable energy and mitigating pollutants. Various support materials such as reducible or non reducible metal oxides, carbon or doped carbon based materials and several mesoporous materials have been used to anchor the several inorganic nanoparticles. Though, these support materials greatly modify the catalytic properties of anchored/supported metal NPs through strong metal support interactions, however, these support materials often block the active sites and prevents the available active sites for the reactant molecules, which not only affects the catalytic activity and selectivity and also difficult to access or elucidate the active sites and interface structure of respective supported catalysts for a chosen reactions. This ultimately leads to the challenges to the catalysts scientist to design the novel nanomaterials catalysts for a industrially relevant reactions. In this regard, I will lightly shed on the advance development of several novel methods for the development of supported catalysts and their applications toward the novel organic transformation reactions. I will also discuss polymer supported metal NPs catalysts and how polymer support could provide as an model support to understand the structure of interfacial and active sites, which guides the rational design of advanced supported nanocatalysts system for a meaningful applications.

Sulfated titania (TiO_2-SO_4^{2-}) as an efficient catalyst for the synthesis of highly functionalized piperidines, benzylamino coumarins and piperidin-4-one oxime derivatives

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ABSTRACT

Sulfated titania (TiO_2-SO_4^{2-}) is a unique and versatile catalytic material which is non-toxic, non-corrosive, non-pollutant and easily separable in nature. As it contains both Lewis acid and Bronsted acid sites. Sulfated titania was engaged in various organic reactions like synthesis of highly functionalized piperidines, benzylamino coumarins and piperidin-4-one oxime derivatives. Sol-gel method was employed for the synthesis of catalyst and confirmed by FT-IR, SEM, TEM, XRD, and EDS characteristic analysis. The pseudo five-component reactions of aromatic aldehydes, aromatic amines, and *β*-keto esters catalysed by sulfated titania (TiO_2-SO_4^{2-}) in methanol at 70ºC provided highly functionalized piperidine derivatives in good to excellent yields. Synthesis of a series of benzylamino coumarin derivatives was carried out *via* the multicomponent reactions of 4-hydroxycoumarin, aromatic aldehyde and cyclic secondary amine in water was obtained using sulfated titania (TiO_2-SO_4^{2-}) as a heterogeneous solid acid catalyst under microwave irradiation at 100°C. The conversion of 2,6-diarylpiperidin-4-ones into their respective oximes in the presence of hydroxylamine hydrochloride was also catalysed by nano-size sulfated titania (TiO_2/SO_4^{2-}) solid superacid. The structure of the all the compounds were confirmed by melting points, elemental analysis, IR, ^{1}H, and ^{13}C NMR and 2D NMR spectral data and single crystal X-Ray analysis. Thus sulfated titania (TiO_2-SO_4^{2-}) gives an good to excellent yield with short reaction time and is inexpensive, easily recyclable catalytic material for this reaction.

Oral/Poster Presentation ABSTRACTs

Curcumin and indole-3-carboxaldehyde derivative: Quantum chemical studies, ADMET and molecular docking studies of SARS-CoV2

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ABSTRACT

SARS-CoV-2 is the designation given to the extremely contagious virus COVID-19 by the International Committee of the Taxonomy of Viruses. Numerous scientific communities from around the world are investigating the lifespan of this recently discovered virus. The development of innovative therapeutic drugs is the subject of numerous various investigations. One of the biggest challenges is understanding how the interactions between the SARS-CoV-2 and drug ligand work. Researchers have discovered the structures of proteins involved in the viral life cycle in the RCSB PDB. In this study, we employed molecular docking study of 1,7-bis(4-hydroxy-3-methoxyphenyl)-4-(1H-indol-3-ylmethylidene)hepta-1,6-diene-3,5-dione (IMBDD) with corona virus proteins (spike protein, spike binding domain with ACE2 receptor and Main protease, RNA-dependent RNA polymerase). Density functional theory calculations were carried out for IMBDD to explore the chemical-reactive parameters. With the aid of Swiss ADME and Osiris data warrior tools, ADMET analysis was carried out in order to analyse the behaviour of IMBDD in a living body and determine the physicochemical characteristics. Additionally, IMBDD toxicity was predicted using online software called pkCSM. Here, we introduce a powerful therapeutic compound that binds to the COVID-19 proteins based on the molecular docking research.

Keywords: COVID-19, Molecular docking, DFT, ADMET, Main protease.

Synthesis and biological evaluation of Nickel (II) complexes of Schiff base ligand derived from 3-Ethoxy salicylaldehyde and 4-phenyl thiosemicarbazide

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ABSTRACT

Schiff's bases, which commonly contain the azomethine group (-C=N-), have been created by condensing primary amines with active carbonyls. Through condensation of 3-Ethoxy salicylaldehyde and 4-phenyl thiosemicarbazide, a novel Schiff base ligand with a flexible coordination behaviour of Nickel (II) complex [Ni($C_{16}H_{15}N_3O_2S$) ($C_{18}H_{15}P$)] has been created and characterised by 1HNMR, X-ray crystallography, IR, and UV-Visible spectroscopy investigations. Based on X-ray crystallographic studies, a distorted tetrahedral coordination structure made up of the N, S, and O of the tridentate thiosemicarbazide ligand and the P atom of the triphenyl phosphane ligand has been proposed for the Ni (II) complex. Moreover, positive outcomes for the antimicrobial screening, particularly for the ligand against bacteria, have been noted. The new Schiff base ligand demonstrates stronger activity towards the Ni (II) metal complex when compared to the reference medication Cyclophosphamide, according to cancer cell line tests of the ligand and their Ni (II)complex on an MCF-7 (Human non-metastatic mammary gland adreno carcinoma) canc93er cell line.

Keywords: *Thiosemicarbazone ligand, Ni (II) complex, crystal structure, biological studies.*

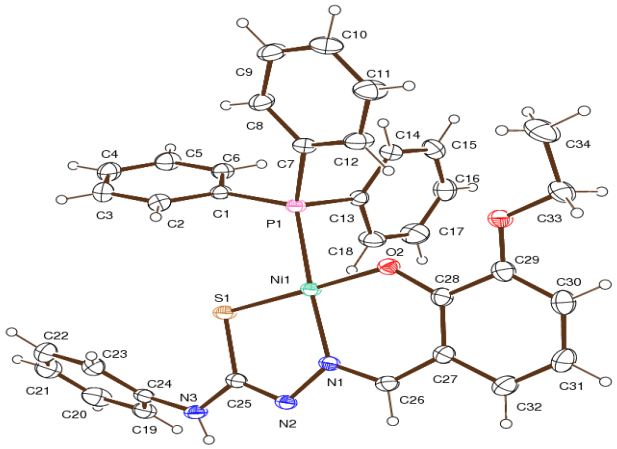

Figure: Labeled ORTEP diagram of Ni (II) complex with thermal ellipsoids at 50% probability

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Iron oxide nanoparticle core-shell magnetic microspheres: Applications toward targeted drug delivery,

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ABSTRACT

This study describes a sensitive reactive oxygen species (ROS)-responsive lecithin (LEC) incorporated iron oxide nanoparticle (Fe_3O_4NP) system with potent anti-inflammatory properties and even more so when the antioxidant drug curcumin (CUR) is encapsulated in the PLGA hybrid magnetic microsphere system (Fe_3O_4@LEC-CUR-PLGA-MMS). The delivery system is responsive to ROS including an H_2O_2 environment to release the payload (CUR) drug. Greater cytotoxicity properties were observed in the presence of Fe3O4@LEC-CURPLGA- MMS against A549 and HeLa S3 cells with IC50 values after 24 h of 10 and 12 μg/mL and 10 and 20 μg/mL, respectively. The present Fe_3O_4@LEC-CUR-PLGA-MMS system demonstrated much better in vitro cytotoxicity, cellular morphological changes and moreover an ability to limit colony formation for A549 and HeLa S3 cancer cell lines than non-cancerous cells, and thus, should be further studied for a wide range of medical applications.

Keywords: Poly(D, L-lactide-co-glycolic acid); Lecithin; Magnetic core microsphere; Cytotoxicity; Targeted drug delivery

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An anti-inflammatory controlled nano drug release and pH-responsive poly lactic acid appended magnetic nanosphere for drug delivery applications

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ABSTRACT

The drug delivery based on reactive oxygen species (ROS) sensitive saponin (SA) layered magnetic iron oxide nanoparticles (Fe3O4 NPs) containing curcumin (CUR) encapsulated in PLA-PVA magnetic nanospheres (Fe3O4@SA-CUR-PLA-MMS) were synthesized and reported in this research article. The prepared nanospheres were characterized through various spectroscopic techniques such as Fourier Transform Infrared (FTIR), X-ray diffractometer (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Thermogravimentric Analysis (TGA) analysis. Drug release profiles demonstrated that the Fe3O4@SA-CUR-PLA-MMS released Curcmin (CUR) based on pH, even in the presence of ROS and hydrogen peroxide (H2O2). Under slightly acidic environments of pH 5.2–7.4, the ROS-responsive polymeric nanocarriers were present in the drug release of CUR from Fe3O4@SA-CUR-PLA-MMS that was pH-induced. Further, Fe3O4@SA-CUR-PLA-MMS showed better cytotoxic properties as well as inhibited colony formation from model cancer cells including HeLa and A549 cells with IC50 values of 12.2 and 11.7 μg/mL respectively, at 24 h. Further proof of the prepared nanospheres cytotoxic activitiy towards cancer cells at 15 μg/mL for 24 h was supplied by fluorescence microscopy images obtained with the aid of AO/EB. MTT assays, fluorescence labeling microscopy, and colony formation assays suggested that the Fe3O4@SA-CUR-PLA-MMS might be a viable anticancer drug for numerous biomedical applications. In conclusion, the current in vitro study presents a potent nanostructured-based approach for enhanced cancer theranostics that has to be further investigated.

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Promising anticancer activity with high selectivity of DNA/plasma protein targeting new phthalazin-1(2H)-one heterocyclic scaffolds

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ABSTRACT

There is a crucial requisite to develop new anticancer agents with significant activity to combat cancer which has infected millions worldwide causing a
n enormous number of deaths. Therefore, in this con- text, new phthalazin-1(2H)-one nucleus containing heterocyclic scaffolds, 2-(4-chloro-1-oxophthalazin- 2(1H)-yl)-N-((1s,4s)-4-hydroxycyclohexyl) acetamide (Z-OP) and 2-(4-chloro-1-oxophthalazin-2(1H)-yl)- N-((1r,4r)-4-hydroxycyclohexyl)acetamide (E-OP), with potent anticancer activities were formulated and characterized here. Results showed that E-OP exhibited promising DNA and plasma protein targeting ef- ficacy greater than that of Z-OP, due to its highly symmetrical structural arrangement. Based on these inspirational results acquired from DNA/plasma protein binding studies, Z-OP and E-OP were systemati- cally investigated for their anticancer activity against human lung carcinoma (A549) and T-cell leukemia (jurkat) cells using MTT assays. Importantly, Z-OP (IC 50 = 4.3 μg/mL) and E-OP (IC 50 = 17 μg/mL) revealed efficient cytotoxicity properties toward the jurkat (IC 50 = 4.3 μg/mL for Z-OP; 4.3 μg/mL for E-OP) and A549 cells (IC 50 = 31 μg/mL for Z-OP; 17 μg/mL for E-OP), relative to their parent compound L4. Fur- ther, Z-OP and E-OP exhibited selective cytotoxicity and safety profiles, as validated using normal human lung (IMR-90) cells (IC 50 > 100 μg/mL for both Z-OP and E-OP). As a part of this study, the drug-likeness, absorption, distribution, metabolism, and excretion (ADME) attributes, as well as in silico toxicity risk as- sessment for Z-OP and E-OP were established. The results from this study provide a new direction for the development of bioactive heterocyclic scaffolds for future clinical trials to once and for all fully succeed in cancer treatment.

Keywords: Heterocyclic scaffolds, DNA targeting, Plasma protein binding, Molecular docking, Selective anticancer activity

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Synthesis, characterization, DNA-binding and cleavage studies of polypyridyl copper(II) complexes

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ABSTRACT

Six new mixed-ligand copper(II) complexes were synthesized namely $[Cu(phen)_2OAc]ClO_4$_H2O(1), $[Cu(bpy)_2OAc]ClO_4$_H_2O(2), [Cu(o-ampacac)(phen)]ClO_4(3), [Cu(o-ampbzac)(phen)]ClO_4(4), [Cu(o-ampacac)(bpy)]ClO_4(5), and [Cu(o-ampbzac)(bpy)]ClO_4 (6) (phen = 1,10-phenanthroline, bpy = 2, 20-bipyridine, o-ampacac = (Z)-4-(2-hydroxylamino)pent-3-ene-2-one,o-ampbzac = (Z)-4-(2-hydroxylamino)-4-phenylbut- 3-ene-2-one) and characterized by UV–Vis, IR, EPR and cyclic voltammetry. Ligands were characterized by NMR spectra. Single crystal X-ray studies of the complex 1 shows Cu(II) ions are located in a highly distorted octahedral environment. Absorption spectral studies reveal that the complexes 1–6 exhibit hypochromicity during the interaction with DNA and binding constant values derived from spectral and electrochemical studies indicate that complexes 1, 2 and 3 bind strongly with DNA possibly by an intercalative mode. Electrochemical studies reveal that the complexes 1–4 prefer to bind with DNA in Cu(I) rather than Cu(II) form. The shift in the formal potentials E1/2 and CD spectral studies suggest groove or electrostatic binding mode for the complexes 4–6. Complex 1 can cleave supercoiled (SC) pUC18 DNA efficiently into nicked form II under photolytic conditions and into an open circular form (form II) and linear form (form III) in the presence of H_2O_2 at pH 8.0 and 37 °C, while the complex 2 does not cleave DNA under similar conditions.

KEYWORDS: Cu(II) complexes; DNA interaction; DNA cleavage; Crystal structure

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Synthesis, physicochemical characterization and structural studies of new Schiff base ligand and its metal (II) complexes: In silico molecular docking analysis, antimicrobial activity and cytotoxicity

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ABSTRACT

A new Schiff base ligand, namely 2-((4-(diethylamino)phenylimino)methyl)-4,6-di-tert-butylphenol (HL), and its derived metal (II) complexes [Cu (L)2] (1), [Co (L)2] (2) and [Zn (L)2] (3) have been synthesized and characterized using various physicochemical techniques. Single-crystal X-ray diffraction studies confirm the structure of newly synthesized HL and complex 2. Density functional theory analysis was used to investigate their electronic structures and properties. In silico docking analysis revealed that complex 1 has significant DNA binding ability (atomic contact energy of −1008.26 kcal mol−1) and complex 2 has a greater affinity with human serum albumin (binding energy of −901.61 kcal mol−1). Complex 2 reveals the highest antimicrobial activity against both fungi and bacteria, whereas complex 1 shows greater cytotoxicity (IC50 = 14.3 ±0.9 μg ml−1) to MCF-7 cancer cells.

KEYWORDS: Antimicrobial activity, Cytotoxicity, in silico docking analysis, metal (II) complexes, Schiff base ligand

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Preparation of mannich base of Cu and Zn complexes with ligand, 2-methoxy-6-((2-(4-(trifluoromethyl) pyrimidin-2-yl)hydrazono)methyl)phenol (HL) for Application in Biological activities

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ABSTRACT

A new Novel mannich base ligand from nicotinamide of copper and Zinc complexes with have been synthesized and characterized and screened for their antimicrobial, antioxidant and DNA binding (in vitro) activities. Their structural features have been established on the basis of analytical, magnetic, conductance, FT-IR, UV-visible, Mass, NMR spectra of synthesized compounds were recorded and discussed. On the basis of color, magnetic moments and electronic spectral data, the square planner geometries of Copper (II) and Zinc (II) complexes have been assigned. The Density functional theory calculations have been performed to gain insights into the electronic structure of these ligand and metal complexes. Antimicrobial activity result shows that, Ligand and complexes copper and Zinc have good antimicrobial agents against (*Escherichia coli*, *Staphylococcus aureus*) and fungi (*Candida species*, *Aspergillus specie*) than others bacterial and fungal strains. Antioxidant activity assay results suggest that, Ligand and complexes of copper and Zinc possess good radical scavenging activity against various free radicals (DPPH). The antimicrobial studies show that the Copper (II) complex is good active than ligand and Zinc (II) complex.

Keywords Mannich base; metal complexes; geometry; antimicrobial activity

Facile green synthesis of MnO_2 Nanoparticles using *Psidium Guajava* extract for the evaluation of photocatalytic degradation of Rhodamine-B and crystal violet dyes

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ABSTRACT

In this work, a simple, efficient and eco-friendly procedure for the green synthesis of manganese dioxide (MnO_2) nanoparticles by Psidium Guajava leaf extract is described. The MnO_2 nanoparticles were synthesized using *Psidium guajava* leaf extract as reducing and stabilizing agents, respectively. Fourier-transform infrared spectrum results revealed the involvement of the functional groups of plant extract in the formation of MnO_2 nanoparticles. The ultraviolet–visible absorption spectra of the synthesized MnO_2 nanoparticles exhibited absorption peaks at 410 nm, which were attributed to the band gap of the MnO_2 NPs. Crystal phase identification of the MnO_2 nanoparticles was characterized by X-ray diffraction analysis and the formation of crystalline MnO_2 nanoparticles has been confirmed. Also, the X-ray diffraction pattern displayed that the average size of MnO_2 nanoparticles was about 80 nm. Furthermore, field emission scanning electron microscopy analysis showed that the synthesised MnO_2 nanoparticles have a spherical shape. MnO_2 nanoparticles have photocatalytic activities for the dye degradation in the visible light region. The photocatalytic activities for the dye degradation of MnO_2 nanoparticles were evaluated using Rhodamine-B and crystal violet as an organic contaminant.

Photodegradation of Methylene blue favored by natural daylight on Fe/ZnO/SiO_2 Nanoparticles catalysts

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ABSTRACT

Photocatalysts have been paid great attention owing to their excellent performance in the degradation of dangerous organic pollutants. Here in, a novel longitudinally grown Fe/ZnO/SiO_2 photocatalyst was made by hydrothermal manner, which had powerful UV-Visible light absorption, and feeble near-IR absorption. The Fe/ZnO/SiO_2 photocatalyst showed tremendous outcomes in the better degradation of methylene blue in trade. The photo-thermal consequence is mostly answerable for the degradation of color under natural sun light irradiation. The Photocatalytic action of Fe/ZnO/SiO_2 catalytic agent in the presence of visible-light irradiation for the degradation of methylene blue was assessed. The consequence of pH, expose time in the presence sunlight, dosage of catalyst loaded, and primary dye concentration on the degradation efficiency of methylene blue was investigated. The results reveal that the optimum photocatalytic oxidation conditions of methylene blue are as follows: pH = 4 and enlightenment time is 5 hrs., the amount of catalyst loading is 7 mg/L and 10% methylene blue dye concentration. Under these conditions, the removal efficiency of methylene blue was 80 – 85%.

Key words: Daylight, Methylene blue, Nanoparticle, Photodegradation, Fe/ZnO/SiO_2

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Synthesis, characteristics and antimicrobial activity of ZnO nanoparticles by using *Triphala Suran* powder

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ABSTRACT

Green technology is the use of diverse plant resources to increase the bioavailability of metal nanoparticles without the use of damaging treatments. The current work focuses on the environmentally friendly production of ZnO nanoparticles employing zinc acetate dihydrate and *Triphala Suran* powder extract as biomolecules. ZnO nano was created using a quick, easy, and environmentally friendly process. X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy were used to analyse zinc oxide nanoparticles (EDX). The existence of ZnO bonding and the adsorption of surfactant molecules on the surface of ZnO nanoparticles were verified by FTIR spectra. A well diffusion approach was used to test the antibacterial activity of ZnO nanoparticles against pathogenic organisms such as Klebsiella pneumoniae, Staphylococcus aureus, Candida albicans, and Penicillium notatum.

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Synthesis, Spectral Characterization, Antimicrobial and Antioxidant Activity of Mixed Ligand Ni(II) complex using Pyrimidine Derivative

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ABSTRACT

This article reports the synthesis and its structural elucidation of pyrimidine based mixed ligand nickel(II)complex. The pyrimidine derivative Schiff base (**HL**) is prepared by the condensation of 2-amino-4,6-dimethyl pyrimidine and 5-nitrosalicylaldehyde. The pyrimidine derivative Schiff base is converted into mixed ligand nickel(II) complex by the addition of 1, 10-phenanthroline and nickel(II) acetate. The prepared pyrimidine derivative Schiff base and complex are structurally pigeonholed by analytical and spectroscopic techniques such as elemental analysis, conductometric measurements, UV-Visible spectroscopy, Fourier Transform Infrared spectroscopy, ^{1}H-NMR spectroscopy, EI-mass spectroscopy. According to the findings, the hypothesised structure of prepared complex has a square planar shape. The stoichiometry of the complex was confirmed as [NiL(phen)](OAc) where, **HL** = 2-(4,6-dimethylpyrimidin-2-ylimino)methyl-4-nitrophenol, (phen) =1,10-phenanthroline and OAc = acetate. Antimicrobial activity of the pyrimidine derivative Schiff base and complex were analyzed by disc diffusion method against various bacterial and fungal strains. A significant inhibition activity was predicted with complex against various bacterial inoculums typed as gram-positive bacteria (*Staphylococcus aureus, Streptococcus pneumoniae, Staphylococcus pneumoniae, Bacillus subtilis*) and gram-negative bacteria (*Shigella flexneri, Salmonella typhi, Klebsiella pneumoniae, Haemophilus influenza*) and various fungal inoculums such as *Aspergillus niger, Candida albicans, Candida tropicalis, Mucor campestris*. The chelating capacity of the pyrimidine derivative Schiff base with Ni(II) ion led to the conclusion that complex is effective antimicrobial agents. Antioxidant activity of pyrimidine derivative Schiff base and nickel(II) complex was analyzed by DPPH assay. Investigation of the antioxidant property of prepared compounds showed that complex has a more antioxidant nature than pyrimidine derivative Schiff base.

Keywords: Pyrimidine derivative; Schiff base; nickel(II) complex; Antimicrobial activity; Antioxidant activity.

Facile synthesis and characterization of WO_3/g-C_3N_4 Nanocompositie for affinitive Photocatalytic degradation of Crystal Violet

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ABSTRACT

Water contamination has become an increasing environmental problem for humans, because the economy and society have developed rapidly. Photocatalytic approaches have been extensively researched in the field of environmental purification. Transition metal tungstates are a significant family of inorganic materials that has potential applications in a wide range of fields and it is studied for many years. Among these nanoparticles WO_3/g-C_3N_4 some were synthesized by using Precipitation method. Constructing a heterostructure is an effective strategy to reduce the electron–hole recombination rate, which enhances photocatalytic activity, size, phase study, and morphology were investigated using various techniques. Moreover, a structural study shows the decoration of WO_3/g-C_3N_4. The photocatalytic effects of the degradation of CV were assessed, and its outstanding capability as a photocatalyst under UV light was noticed throughout the investigation. The WO_3/g-C_3N_4 was characterized by using FESEM, XRD, FTIR, UV–DRS, The powder XRD analysis showed crystal structure, and SEM images show surface morphology due to their crystalline/amorphous combination. FTIR analysis confirms the nature of the interaction between organic and inorganic counterparts. UV optical spectra exhibit a blue-shifted absorption band/increased band gap nature due to their crystalline formation. The PL emission spectrum shows an enhanced emission band, indicating that the presence of organic molecules reduces or controls the size of defects. The photocatalytic efficacy against the CV was followed by first-order reaction kinetics, with a maximal degradation efficiency of 77% within 60 min.

Keywords: Photodegradation, Crystal violet, Nanocomposite

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Nanostructured Bismuth tungstate for the Efficient Photocatalytic Degradation of MB under UV-light Irradiation

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ABSTRACT

The layered crystal structures and electronic band topologies of Bismuth-based photocatalysts have prompted a significant amount of anxiety. In this work, the hydrothermal method was used to synthesize the Bi_2WO_3 photocatalyst. X-ray diffraction, Fourier-transform infrared spectroscopy, scanning electron microscopy, and Photodegradation studies were used to characterize the morphology, crystal structure and photocatalytic properties of the Bi_2WO_3. MB solution (100 mL, 20 mg/L) was degraded by 20 mg Bi_2WO_3 within 60 minutes with a mineralization rate of 80%. From the photodegradation studies, hydrothermally synthesized Bi_2WO_3 facilitated the transport of electron-hole pairs and their separation. Furthermore, the mechanism and degradation pathways of MB photodegradation were presented. This paper presents a novel method for designing additional Bi-based photocatalysts with superior photocatalytic capabilities. It also discusses an effective catalyst for the removal of MB from water.

Keywords: Bismuth Tungstate, Photodegradation, Methylene Blue Nanocomposites

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Evaluation of photocatalytic activities of visible-light driven green synthesis MnO_2 nanoparticles using *Clerodendrum phlomidis* extract

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ABSTRACT

Manganese oxide (MnO_2) nanoparticle were fabricated through green route using *Clerodendrum phlomidis* extract. The green synthesis MnO_2 nanoparticles were characterized by UV-Vis, XRD, EDX, SEM and XPS techniques. Moreover, the photocatalytic effects of MnO_2 nanoparticles on the degradation of Methylene blue (MB) were assessed, and its outstanding capability as photocatalysis under UV light was noticed throughout the investigation. This is a 100% environmentally friendly method that does not employ any harmful or hazardous solvents. The adopted green rout furnished semi spherical MnO_2 nanoparticles, uniformly distributed and particle size in the range of 10 nm. The synthesized MnO_2 nanoparticles showed excellent photocatalytic activity against Methylene blue under UV light irradiation and maximum degradation of 80.99 % was achieved with 60 min of reaction time. In view of promising activity, the MnO_2 nanoparticles could be used photocatalyst for the degradation of dyes in wastewater and *Clerodendrum phlomidis* extract can be applied as eco-benign and cost effective approach for MnO_2 nanoparticles synthesis. As a result, the biosynthesized MnO_2 nanoparticles synthesized from *Clerodendrum phlomidis* extract to have the potential to be used in photocatalytic applications.

Keywords: *Clerodendrum phlomidis*, Manganese dioxide, Methylene blue dye

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Synthesis, Characterization, and Antimicrobial Activities of Copper Oxide-Embedded Banana Fiber for Food Packaging Materials

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ABSTRACT

Food packaging plays a crucial role in preserving the quality and safety of food products. However, the widespread use of synthetic packaging materials has led to environmental concerns due to their non-biodegradable nature. Therefore, there is a growing demand for eco-friendly packaging materials that can replace traditional synthetic materials. In this study, we investigated the potential of copper oxide-embedded banana fiber as a sustainable and effective food packaging material with antimicrobial properties. The synthesis of the composite material involved immersing banana fiber in a copper oxide solution. The resulting composite material was characterized using various analytical techniques such as scanning electron microscopy (SEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR). SEM images revealed that the copper oxide nanoparticles were well-dispersed on the surface of the banana fiber. XRD analysis confirmed the presence of copper oxide in the composite material, and FTIR spectra showed that there was no significant chemical interaction between the copper oxide nanoparticles and the banana fiber. The antimicrobial activity of the copper oxide-embedded banana fiber was evaluated against two common food-borne pathogens, Escherichia coli and Staphylococcus aureus. The disc diffusion method was used to determine the inhibition zones, which indicated the effectiveness of the composite material against the tested microorganisms. The results showed that the copper oxide-embedded banana fiber exhibited excellent antimicrobial activity against both bacteria, with inhibition zones of 13.2 mm and 14.5 mm for *E. coli* and *S. aureus*, respectively. This suggests that the composite material has the potential to prevent the growth of food-borne pathogens in food packaging applications. In addition to its antimicrobial properties, the mechanical and physical properties of the composite material were also evaluated. The tensile strength and Young's modulus of the composite material were determined using a universal testing machine. The results showed that the copper oxide-embedded banana fiber had good mechanical properties, with a tensile strength of 18.2 MPa and a Young's modulus of 1.9 GPa. The water vapor transmission rate (WVTR) of the composite material was also determined using a gravimetric method. The WVTR value was found to be 5.4 g/m^2/day, which is within the range of commercially available food packaging materials. Overall, the results of this study demonstrate the potential of copper oxide-embedded banana fiber as a sustainable and effective food packaging material with antimicrobial properties. The composite material exhibited excellent antimicrobial activity against common food-borne pathogens and had good mechanical and physical properties. This suggests that the material can potentially replace traditional synthetic packaging materials and reduce environmental pollution. However, further studies are needed to investigate the long-term stability and biodegradability of the composite material in different environmental conditions.

Synthesis, Characterization, and Biomedical Applications of Graphene-Folic Acid Nanoparticles Doped with Copper Oxide Nanoparticles

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ABSTRACT

Graphene has been widely studied for its unique properties, such as high mechanical strength, high electrical conductivity, and large surface area, making it a promising material for biomedical applications. In this study, we report the synthesis, characterization, and biomedical applications of graphene-folic acid nanoparticles doped with copper oxide nanoparticles. The nanoparticles were synthesized through a facile one-step hydrothermal method using graphene oxide, folic acid, and copper acetate as precursors. The resulting nanoparticles were characterized using various techniques, including X-ray diffraction, transmission electron microscopy, scanning electron microscopy, Fourier-transform infrared spectroscopy, and Raman spectroscopy. The results showed that the nanoparticles were successfully synthesized and had a uniform size distribution with an average diameter of 50 nm. The biomedical applications of the nanoparticles were evaluated in vitro using human breast cancer cells (MCF-7). The nanoparticles exhibited excellent biocompatibility and low cytotoxicity, indicating their potential for biomedical applications. Furthermore, the nanoparticles were found to have a high cellular uptake, which can be attributed to the presence of folic acid, which targets cancer cells that over-express folate receptors. The copper oxide doping of the graphene-folic acid nanoparticles was found to enhance their antibacterial activity. The nanoparticles showed excellent antibacterial activity against both Gram-positive and Gram-negative bacteria, including Escherichia coli and Staphylococcus aureus. The antibacterial activity was attributed to the release of copper ions from the nanoparticles, which disrupt the bacterial membrane and cause cell death. In conclusion, the graphene-folic acid nanoparticles doped with copper oxide nanoparticles synthesized in this study exhibited excellent biocompatibility, low cytotoxicity, high cellular uptake, and enhanced antibacterial activity. These properties make them promising candidates for biomedical applications, including targeted drug delivery and antibacterial therapy. Future studies will focus on evaluating the in vivo efficacy and toxicity of these nanoparticles to further validate their potential for clinical use.

Pyrimidine derived imine capped nickel nanoparticles for catalytic activity in dye degradation and bacterial-resistant colorization of cotton

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ABSTRACT

Nanotechnology has emerged as a promising field for the development of new materials with advanced properties and applications. In this study, we synthesized pyrimidine-derived imine-capped nickel nanoparticles (NiNPs) using a simple and cost-effective method. The obtained NiNPs were characterized using various techniques such as UV-visible spectroscopy, transmission electron microscopy, X-ray diffraction, and Fourier-transform infrared spectroscopy, which confirmed the successful synthesis of the nanoparticles. The synthesized NiNPs were evaluated for their catalytic activity in the degradation of dyes commonly used in the textile industry. The results showed that NiNPs exhibit excellent catalytic activity and efficiency in the degradation of dyes, with more than 90% of the dye being degraded within a short period. The catalytic activity of NiNPs was found to be dependent on the size and concentration of the nanoparticles. Furthermore, the NiNPs were also used for bacterial-resistant colorization of cotton fabrics. Cotton fabrics were treated with NiNPs, and the antibacterial activity of the treated fabric was evaluated against two common bacteria strains, namely Staphylococcus aureus and Escherichia coli. The results showed that the NiNPs-treated cotton fabrics exhibit excellent antibacterial activity against both strains, with more than 99% of bacterial growth inhibition. Overall, this study demonstrates the potential of pyrimidine-derived imine-capped nickel nanoparticles as a highly efficient and cost-effective catalyst for the degradation of dyes and as a promising antibacterial agent for the colorization of cotton fabrics. The findings of this study could have significant implications for the development of advanced materials with unique properties and applications in various fields, including textile manufacturing, environmental remediation, and biomedical applications.

Enhancement of wound healing using Olive based nano type band aids

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ABSTRACT

Skin is the first line barrier in defense against infections. The breaking of skin permits the entry of bacteria. This infection may shift the wound to a chronic condition since it is not healed within the stipulated period. This delayed process of healing is due to infection, poor circulation and nutrition. Our aim of the study is to develop a natural polymer-based thin film incorporating olive oil for the wound healing process.

Hydroxyapatite with cellulose acetate immersed in olive oil used for thin film development. The polymer cellulose acetate acts as nano pillar to enhance the surface area for adhesion. The added olive oil helps to restrict the water absorption and promote the antibacterial activity along with the enhancement of mechanical properties. These modified thin films were characterized using FTIR to confirm the range of functional groups and deduce the molecular structure. Further this helps to find out the chemical composition and physical state of the developed thin film. Experimental results showed that increasing the percentage of olive oil in cellulose acetate membranes increases the antimicrobial activity against Escherichia coli (E. coli).The comparison of the film developed with and without olive confirms that the antibacterial activity induced in the sample is only due to olive and this can be used as novel band aid for wound healing process. This developed film provides sufficient oxygen and nutrient for quick heal. Therefore the newly prepared CA/HAp immersed olive oil nano composite thin film can be used as a promising antibacterial and wound healing dressing for rapid and efficient recovery.

Keywords: HAp, Cellulose acetate, olive oil anti-bacterial activity and anti-oxidant activity

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Natural polymer Electrolyte with magnesium chloride hydroxide using super capacitor application

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ABSTRACT

In the current situation the energy demand is fulfilled due to the advancement of electrochemical devices like fuel cells, batteries, and supercapacitors. A biopolymer electrolyte made of a Gellan Gum blend with PVA and magnesium chloride (MgCl2) has been created using the solution casting method. It is environmentally benign, low-toxic, and biodegradable. In the current study, biopolymer electrolytes were created using a $MgCl_2$ salt compositions at varying concentrations. X-ray diffraction analysis was used to analyses the produced biopolymer electrolytes (XRD), Fourier Transform Infrared (FTIR) spectroscopy used to define complex formation of the polymer electrolyte, Different Scanning calorimetric (DSC) is a technique we use to study thermal stability of the biopolymer electrolytes. The highest ionic conductivity has been found by 0.5g of gellan gum and 0.5g of PVA with 0.4g of $MgCl_2$ from the plots of Cole–Cole analysed at different temperatures for the higher conducting polymer electrolytes.

Keywords: Biopolymer Gellan gum, poly vinyl alcohol (PVA), $MgCl_2.6H_2O$ Salt, DSC, Electrochemical Properties

Synthesis, Characterization, and Electrochemical Studies of copper (II) Schiff base Complexes and their *Electrocatalytic determination of 4-nitrophenol*

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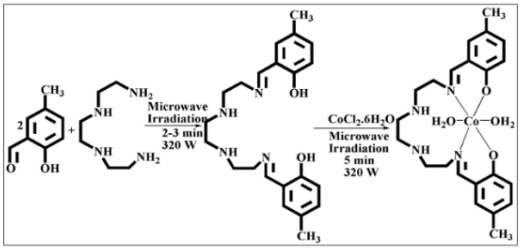
ABSTRACT

Aromatic nitro compounds are widely used in industries for the synthesis of pesticides, synthetic dyes, pharmaceuticals, paints, and petrochemical products [1]. The nitro compounds add undesirable color to water resources, preventing the penetration of sunlight, retarding photosynthetic reactions, and affecting aquatic life and pose serious detrimental effects to living beings and plants. 4-nitrophenol (4-NP) is one of the most detrimental among various nitro compounds. It has been reported as a potential carcinogen, mutagen, and teratogen. It also causes severe headaches, drowsiness, nausea, and cyanosis. Hence, its utilization requires strict control and monitoring to avoid adverse effects on living beings. Therefore, a simple and accurate analytical method is necessary for the measurements of 4-NP. Several methods have been developed, such as capillary zone electrophoresis, HPLC, gas chromatography (GC), fluorescence, and spectrophotometry [2]. However, the electrochemical technique usually offers greater sensitivity, in addition to its other outstanding features such as low cost, easy operation, fast response time, and great potential for miniaturization and construction for portable equipment applications [2]. In the present work, we have successfully employed the copper (II) Schiff base complex modified GCE for the determination of 4-NP. Thus, an electrochemical sensor was prepared by simply electrochemical polymerization at a glassy carbon electrode (GCE) for the detection of 4-NP. The fabricated 4-NP sensor exhibited excellent sensitivity and selectivity. It can be used for real sample analysis.



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Prospects of Phyconanotechnology-Seaweeds as a Potential Source of Biomaterials.

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ABSTRACT

In recent times, bio-based nanoparticle synthesis has become a novel technique with a minimal toxic effect in medical fields. Among the different biological sources, Marine algae plays a significant role in the synthesis of nano biomaterials. As a rich source of natural bioactive compounds- phytochemicals, PUFA, antioxidants, polysaccharides, aminoacids, vitamins and minerals, seaweeds are of nutritional significance and can be used as an alternative food source. Seaweeds are great suppliers of many nutrients despite their enormous diversity in terms of its species and environmental factors. In comparison to plants and other food sources, seaweeds grow at a significantly faster rate. The maritime environment has been shown to be a great source of biological and chemical diversity because of its environmental attractiveness. Based on its pigmentation factors, seaweeds are classified as; rodophyta, chlorophyta and phaeophyta. This study is about understanding phyconanotechnology (algal derived nanoparticles) – where the active metabolites of algal biomass act as a key component in nanoparticle synthesis with a major biochemical property, (antioxidant, antimicrobial and anticancer activity).

Keywords: Nano biomaterials, bioactive compounds, Marine algae, Phyconanotechnology, Biochemical properties

EFFECT ON ELECTRODEPOSITION OF NI-ZN-SIO_2 NANOCOMPOSITE COATINGS TO ENHANCE THE CORROSION RESISTANCE AS COMPARED TO NI-ZN ALLOY

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ABSTRACT

In present study, it is achieved by incorporation of suitable inert particles in the Ni-Fe alloy matrix. Ni-Zn-SiO_2 nanocomposite coatings have higher micro hardness values compared to Ni-Zn alloy coatings due to the incorporation of SiO_2 into the Ni-Zn alloy matrixes. It has changed the microstructure and grain size of the nanocomposite deposits. The X-ray diffraction has confirmed the crystallite size and structure of the pulse electrodeposited Ni-Zn alloy and Ni-Zn-SiO_2 nanocomposite coatings. The average crystallite size calculated from Scherrer formula was 45 nm for Ni-Zn alloy, 43 nm for Ni-Zn-SiO_2 nanocomposite coatings. The co-deposited SiO_2 has reduced the grain size. The surface morphology of both Ni-Zn alloy and Ni-Zn-SiO_2 nanocomposite coatings were examined through Scanning electron microscopy. The Ni-Zn alloy has spherical sized deposits. After the inclusion of SiO_2 particles into the Ni-Zn alloy matrix, the surface morphology was changed into smaller sized deposit. When compared to Ni-Zn alloy matrix, Ni-Zn-SiO_2 nanocomposite coatings have a smooth surface and finer grain particles were distributed. The corrosion resistance behaviour of Ni-Zn-SiO_2 nanocomposite coating was examined through electrochemical impedance measurement studies in 3.5% NaCl solution. The results showed that, the Ni-Zn-SiO_2 nanocomposite coatings have more corrosion resistance than Ni-Zn alloy coatings.

Keywords: Nickel Sulphate, Zinc Sulphate, SiO_2 , Ni-Zn alloy, Ni-Zn-SiO_2 nanocomposite.

BACTERIAL AND FUNGAL DIVERSITY IN THE RHIZOSPHERE REGION OF HERBAL PLANT

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ABSTRACT

The extent of the diversity of microorganisms in soil is considered to be critical in the maintenance of soil health and quality, as a wide range of microbes plays an important role in soil functions. This comparison analysis, in a tiny way, concentrates on the diversification of microorganisms such as bacteria, fungi, and actinomycetes in the soil close to the roots of a herbal plant (*Azadirachta indica*) in the mountainous region. The *Azadirachta indica* tree roots beginning to grow at the top and bottom of the hill were used to collect soil samples. For the growth of bacteria, fungi, and actinomycetes, the soil samples were serially diluted and plated on nutrient agar, potato dextrose agar, and starch casein agar, respectively. 20 distinct bacterial strains, the uphill and downhill regions were separated from the soil samples, and their characteristics were determined using both biochemical and morphological techniques. The findings showed that the rhizosphere of the *Azadirachta indica* tree contained a wide variety of microorganisms. Additionally, molecular research and evaluating the frequently isolated isolates for a variety of bioactivities may provide more clarity on the diversity of microbes and their potential applications.

Keywords: Soil, Diversity, Microorganisms, *Azadirachta indica*, Serial dilution, Biochemical test.

PRELIMINARY ANALYSIS OF MICRO PLASTIC PARTICLES IN WATER BODY IN AGNIYAR RIVER DRAINAGE BASIN AT TANJORE DISTRICT EAST COAST OF INDIA

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ABSTRACT

Microplastics are emerging contaminants in environment that is from fragmentation of large plastic into a small plastic of size below 5mm, which have been prominent since the last decade. This is due to the adverse effect in aquatic ecosystem and due to heavy growth of plastic waste around the world. Mismanaged Plastic particles which end up in the water bodies like rivers, lakes, ocean etc will leads to significant hazards to the environment. The plastic that gets deposited on the water bodies turn into smaller particles of plastics known as micro plastics and there is a high chance of these micro plastics enter into the aquatic ecosystem and human body through various ways. Some of the most common ways are through drinking water and through aquatic animals that we consume. These plastics are said to cause damage to cells (causing cell death) and other various harm to human body. Recent studies have found microplastic in human blood. So, the water bodies from Agniyar river was sampled and tested with FTIR techniques which shows the abundance of expanded plastics have been kinds of polymers <0.05 g cm-3 and low density plastic ranged from 0.90-0.99 g cm-3. The present study confirms that Agniyar River is polluted with microplastics contaminants and need proper mitigation measures before it bring a severe threat to aquatic ecosystem.

Keywords: Microplastics, mismanaged plastic, FTIR techniques, expanded plastics, mitigation measures

CONSTRUCTION OF HEXAGONAL ROD SHAPE OF ZnO WITH ENRICH THE PHOTOCATALYTIC DEGRADATION OF AMOXICILLIN

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ABSTRACT

In this chores the active photocatalyst of ZnO were mainly account for the removal of organic pollutants from waste water and also degrade the industrial wastage of organic pollutant such as drugs, dyes and pesticides. The active photocatalyst ZnO was synthesized by the simple precipitation method. On that occasion the photocatalyst were characterized by various analytical tools including XRD, XPS, UV-Vis-DRS, SEM- EDAX to explore the crystallinity, chemical composition, band gap, surface morphology were deliberated. Especially ZnO photocatalyst has enhance the photocatalytic activity compared to other transition metals which was confirmed by the photocatalytic degradation of Amoxicillin (AMX). The enhanced photocatalytic activity of ZnO not only enhance the light absorbance range but also accelerate the photo induced interfacial charge transfer during the photocatalytic process. Influence factors such as initial dye concentrations and catalyst dosage were also investigated. The organic pollutants were degraded under visible light illumination on ZnO photocatalyst surface. Interestingly 40mg of the catalyst and 10mg/L concentration were optimized condition for the essential photocatalytic degradation of AMX .The hydroxyl radical (·OH) has the most active species involved in the photodegradation of AMX which was scavenge by trapping experiments. Moreover this study also provides a new platform for the degradation of AMX.

Keywords: Hexagonal rod like ZnO, Visible-light Photocatalyst, Amoxicillin.

Synthesis, characterization, and binding optimization studies of V(v) ion-imprinted polymeric gel

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Ion imprinting is a method of imprinting template ions on a polymer matrix. It possesses significant applications in the field of material science including selective sorption, solid phase extraction, sensors, etc. A novel V(v) ion-imprinted polymeric gel(IIPG) based on polyacrylamide and alginic acid was synthesized by the solution polymerization method in the aqueous medium. The synthesized polymeric gel is characterized by FTIR spectroscopy and XRD analysis. The batch equilibration method optimizes the conditions for sorption of V(v) ions such as initial concentration and time of contact. The binding efficiency was estimated using UV-Vis spectrophotometric method and is found to be increased along with an increase in the parameters stated above effectively. Also, the selective affinity of IIPG towards V(v) ions from aqueous solutions was confirmed by competetive adsorption studies with certain metal ions such as Ce(IV), Cr(VI), Zn(II) which were selected randomly.

Keywords: vanadium, IIPG, Sorption

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Highly Selective and Sensitive Electrochemical Dual Object Sensing Platform of Silicon Quantum Dots From Recycled Column silica gel

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ABSTRACT

The selective determination of heavy metals and toxic herbicides in water and soil is of major significance since they are extremely detrimental to the environment and human health. A facile one-step synthetic approach was developed for the fabrication of silicon quantum dots (SiQDs) and used as an electrochemical dual sensor for Cu(II) and 2,4-dichlorophenoxyacetic acid[1]. The structural properties and morphological investigation of the SiQDs were systematically studied by various techniques. This newly designed SiQDs/GCE-based electrochemical sensor can measure an extremely wide range of Cu(II) (0.1-2400 µM) in 0.1M phosphate buffer solution (PBS) with a limit of detection (LOD) 11 nM. The proposed dual sensor was showing highly selective performance to detect possible interference from common interfering substances that are present in water and soil samples. Additionally, the dual sensing behavior of SiQDs providing two chemical inputs (Cu(II) and 2,4-D) helps to construct an INHIBIT logic gate. The as-fabricated SiQDs exhibit several advantages such as rapidity, selectivity, excellent reproducibility, repeatability, and long-term stability for sensing Cu(II) and 2,4-D, which opens a facile analytical platform for environmental applications. To the best of our knowledge, this is the first recycled column silica gel-based SiQDs as an electrochemical dual sensor[2].

Keywords: Silicon quantum dots, electrochemical, sensing, dual sensor

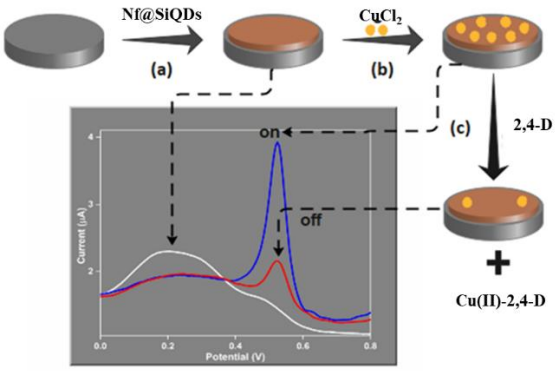

Figure 1: Illustration of electrochemical detection of Cu(II) and 2,4-D with SiQDs

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PVA/Cellulose based biodegradable polymer composite films for packaging applications

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ABSTRACT

The cellulose is the most abundant biodegradable material available in nature. The cellulose finds much more applications in the field of material science, biomedical and electronics. The extraction of cellulose from various sources via various methods were explored by researchers. The major source of cellulose is plants. This work aims at extraction of cellulose from agro waste material, rice husk. A huge quantity of rice husk waste generated every year, which were usually disposed by burning it in open environment. The risk of air pollution caused by its disposal is hazardous to all the living entities. The rice husk was rich in lingo cellulosic content and the extraction of cellulose from this rice husk may pave way for the conversion of agro waste to value added product and avoid pollution of the environment. The rice husk was collected and finely grinded, sieved to uniform size. Then the sieved rice husk was subjected delignification, followed by bleaching process. The bleached materials were hydrolysed to get the cellulose. The cellulose obtained was filtered and dried. Then it was characterised with FTIR to ensure the chemical composition, XRD to finds its crystallinity, SEM to explore its morphology, TGA to finds its thermal stability. The polymer poly vinyl alcohol is water soluble and it is taken as the matrix. The cellulose extracted from rice husk was added to the matrix poly vinyl alcohol as filler material. The solubility of the matrix in water was reduced by the addition of cellulose as filler. There by it serves as a better packaging material, with improved moisture resistance, cheap, affordable and biodegradable.

Keywords: cellulose, rice husk, biodegradable, polymer, matrix, filler

Flexible MWCNT Buckypaper for ThermoelectricApplications

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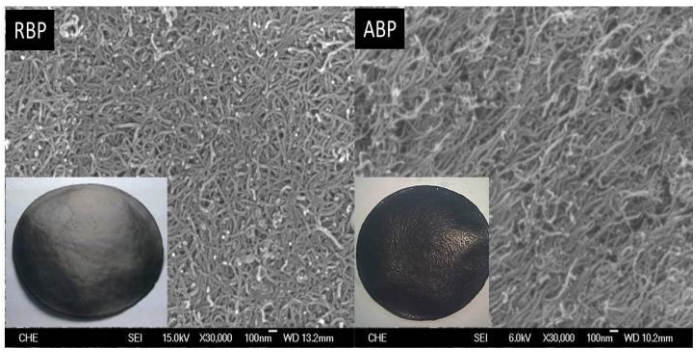
ABSTRACT

Carbon nanotubes (CNTs) have drawn much attention during the last two decades owing to its inimitable structure and astonishing properties. We sufficiently utilized the unique properties of CNTs by making of flexible paper like structure called as buckypaper. Buckypaper (BP), the thin macroscopic freestanding sheets made from aggregation of single or multi-walled CNTs. Here we processed simple method of suspension and filtration to fabricate the random and aligned network of MWCNTs called random-BP (RBP) and aligned-BP (ABP) respectively, displayed below.

We demonstrates the prepared BP by depositing thermoelectric metals (Bi, Te, Sb) and its metal alloys (BiTe, BiSb, SbTe) on BP surface for thermoelectric applications. We measured the electrical resistivity (ρ) and enhanced Seebeck coefficient (S) upto ~22 and ~51 μV/K, to calculate the thermopower ($S^2\sigma$) and its figure of merit (ZT) value ~0.06-0.1. The well-established semiconducting properties combined with mechanical properties of buckypaper, the expected enhancement in the thermoelectric performance was achieved, which is useful for flexible thermoelectric device applications.



The Future Biomass Utilization and Applications

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ABSTRACT

A simple, ecological, and cost-effective method for producing highly porous activated carbons from a variety of natural waste products. The method of activation used in the procedure is either physical or chemical. Several analytical techniques were used to examine its structural, physical, and chemical properties. The as-synthesized metal decorated nanocomposites were used as catalysts, while undoped porous carbons were used as binder-free electrode materials for catalytic, sensors, and supercapacitors applications, with outstanding rate constant, sensitivity, and specific capacitance. The development of an alternative electrode material from bio-waste serves two main purposes: (i) It helps with waste disposal; converting waste into a useful product, and (ii) it provides an economic argument for the substantiality of supercapacitor technology. In addition to this, recent developments in carbon-based materials derived from bio-waste for sustainable sensor, catalytic and energy conversion applications.

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Facile synthesis of nano-Fe_2O_3/montmorillonite nanocomposite with UV-A light photo degradation of Reactive yellow 86 and Acid red 73

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ABSTRACT

In this work, montmorillonite clay modified with nanoparticles of Fe_2O_3 (Fe-Mt) was synthesized to be used as a catalyst for the degradation of Reactive Yellow 86 (RY 86) and Acid red 73 (AR 73). The nanocomposite has been characterized by different methods (XRD, FT-IR, SEM-EDX, TEM and UV–DRS). In aqueous solutions, the performance of the new catalyst has been highlighted in the degradation of RY 86 and AR 73. The degradation efficiency of the RY 86 in a mixture (RY 86 - Fe-Mt - H_2O_2) and AR 73 in mixture (RY 86 - Fe-Mt - H_2O_2) at pH = 7 achieved a 100% removal of RY 86 and AR 73 in 60 min. The formation of iron (III) shows the involvement of the Fenton process, which has been operated at pH = 7. Several parameters that affect this process have been optimized as pH, (Fe-Mt) dosage and H_2O_2 concentration. The reusability of the nanocomposite was examined in several consecutive runs, and the degradation efficiency decreased only below 5% after 4 repeated runs.

Keywords: Montmorillonite, Reactive Yellow 86, Acid red 73, Fenton process

KINETICS AND THERMODYNAMIC STUDIES OF BIOSORPTION OF METHYLENE BLUE FROM AQUEOUS SOLUTION USING CHARCOAL ALGINATE- IRON BEADS

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ABSTRACT

Population explosion and industrial advancements have resulted in a sharp deterioration of several ecosystems, posing serious threats to human health and environment. Several civic bodies have promulgated regulations monitoring the emission of contaminants from industrial waste streams. Among the different pollutants of aquatic ecosystem, dyes are a large and important group of chemicals. It is reported that there are over 100,000 commercially available dyes with a production of over 7×10^5 metric tonnes per year. Dyes are generally believed to be toxic and carcinogenic, or derived from other known carcinogens. The conventional methods for the removal of dyes involve high capital cost with recurring expenses, incomplete metal removal, high reagent and energy requirement and generation of toxic waste products. Among several chemical and physical methods, biosorption process is one of the effective techniques that have been successfully employed for the removal of toxic heavy metals from wastewater.

The present study focused on the removal of methylene blue (MB) from aqueous solution by using charcoal alginate- iron beads. Batch experimental procedure was used for the biosorption study. The prepared biosorbent had much potential as an efficient and useful biosorbent for the removal of MB from aqueous solution.

Biosorption experiments were carried out to study the effect of parameters such as pH, initial concentration, contact time and biosorbent dose on the biosorption process. The residual concentration of MB after treating with bead was determined by spectrophotometer at 665nm. The isotherm study was conducted by using models such as Langmuir and Freundlich. From the isotherm study, Langmuir was found to be the best fit for the removal of MB. The kinetic study was conducted by using pseudo-second-order model. The pseudo-second-order model was found to be better fit for the removal of MB dye. The -ve value of ΔG indicated the feasibility of the process and spontaneous nature of biosorption. The +ve value of ΔH and ΔS indicated the endothermic nature and irreversibility of MB biosorption

The results of the present investigation demonstrate that charcoal alginate- iron beads can be used as an effective and alternative biosorbent for the removal of MB dye from wastewater.

Key words: Biosorption, Methylene Blue, Charcoal alginate-iron beads

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Synthesis, structure, DNA/protein molecular docking and biological studies of hydrazone ligands derived Cu(II) and VO(IV) complexes

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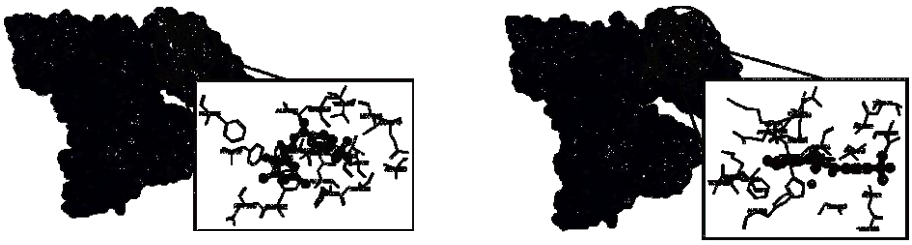
ABSTRACT

In this work, Cu(II) (**1**) and VO(IV) (**2**) complexes are synthesized from hydrazones, HL1=(E)-N′-(2-hydroxy-3,5-diiodobenzylidene)-4-*tert*-butylbenzohydrazide and HL2=(E)-N′-(3-bromo-5-chloro-2-hydroxybenzylidene)-4-*tert*-butylbenzohydrazide and are well characterized by the way of different spectroscopic and analytical techniques. The chemical structure of complexes **1** and **2** is confirmed by single crystal X-ray crystallography studies. The molecular docking studies are carried out to better comprehend the preferential mode of binding of these compounds against biomolecular targets such as DNA and plasma protein (HSA). Complex **1** revealed the lowest ACE value (-503.36 kcal/mol), suggests that the potential DNA binding efficacy of complex **1** is being stronger than the other compounds of interest. Besides, complexes **1** and **2** displayed better binding affinities with HSA protein molecules relative to their respective parent hydrozone ligands. These results have been reflected as their significant antibacterial and antifungal activities.

Keywords: Metal complexes of hydrazone; Crystal structure and Molecular docking



3D interactions of docked conformation of (HL_2) and its (2) (From top to Bottom)

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Maranta arundinacea Leaf Extract for Sustainable Synthesis of Silver Nanoparticles with Efficient Azo Dye Degradation

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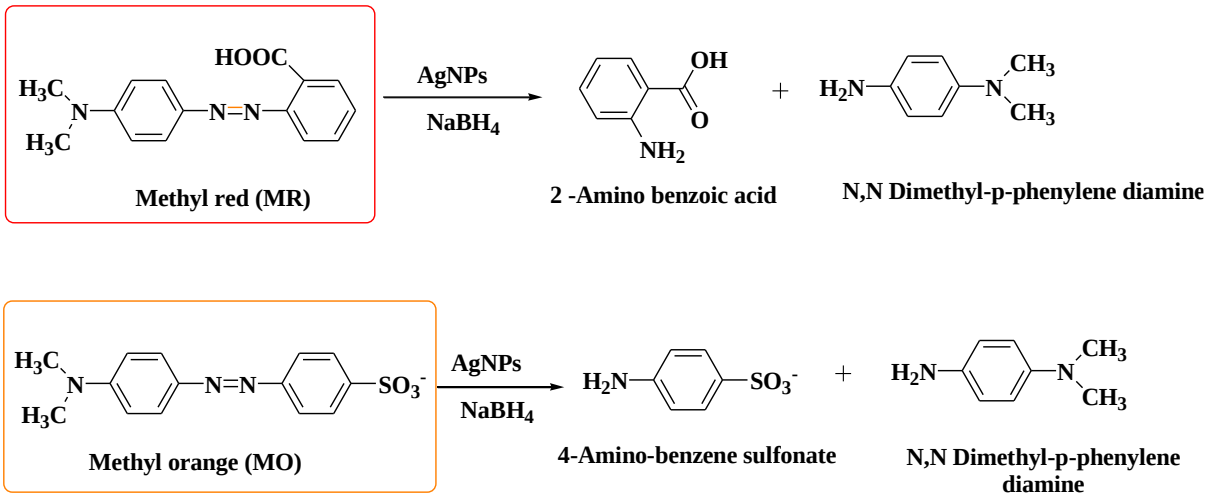
ABSTRACT

The present research work highlights the sustainable and eco-friendly approach for synthesizing silver nanoparticles using *Maranta arundinacea* or West Indian arrowroot, and its potential catalytic applications. The nanoparticles were prepared by reducing silver nitrate with an aqueous leaf extract of *Maranta arundinacea* using microwave irradiation. The synthesis was confirmed through UV-visible spectrophotometer, FT-IR, XRD, DLS, Zeta potential, and SEM-EDX analysis. The nanoparticles showed the presence of hydroxyl groups on their surface, which played a critical role in their capping and stabilization. The optimization conditions of room temperature and the amount of leaf extract were studied, emphasizing the role of microwave irradiation and leaf extract in the synthesis process, respectively. The nanoparticles exhibited anionic behavior, as indicated by the high negative value of Zeta potential. Furthermore, the synthesized nanoparticles demonstrated excellent catalytic activity for the degradation of organic dyes such as methyl orange and methyl red.

Keywords: Azo dyes; *Maranta arundinacea*; Silver Nanoparticles; Green Synthesis; Sustainable Chemistry; Catalytic degradation



Scheme 1: Degradation mechanism of methyl red and methyl orange

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Green Synthesis of Silver Nanoparticles using Extract of *Myristica fragans* Assisted By Microwave Irradiation

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ABSTRACT

Majority of physicochemical methods reported for the synthesis of silver nanoparticles include the use of toxic chemicals and severe reaction conditions which lead to high chemical toxicity and environmental pollution.[1] Hence, the green mode of nanoparticle synthesis via the plant extracts, microorganisms and enzymes are gaining much importance in the present scenario.[2] The green approach by the use of plant extract is a very safe, cost effective and non-toxic method for the silver nanoparticle synthesis. This green synthetic route causes less chemical toxicity and hence is environmentally benign. This method also eliminates the cost and elaborate process of microorganism isolation and maintaining cell cultures.[3] In the present study, the silver nanoparticles were synthesised using aqueous leaf extract of *Myristica fragrans* and silver nitrate solution using microwave assistance. The plant extracts act as both reducing and capping agent.[4] The synthesised silver nanoparticles were characterized using Ultra Violet-visible spectroscopy, Fourier Transform Infrared spectroscopy, X-ray diffraction and High resolution transmission microscopy analysis.

Keywords: Silver nanoparticles, Green synthesis, *Myristica fragrans*, Microwave irradiation

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Synthesis, Characterization and Sorption study of Cr(IV) ion-selective non-crosslinked polymer network

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ABSTRACT

A novel Cr(VI) ion-selective non-crosslinked polymer network(ISNCPN) is synthesized from an aqueous medium. Techniques viz. UV-Visible spectroscopy and FTIR spectroscopy were used to characterize the polymer synthesized. Sorption studies of the ISNCPN were carried out at different conditions such as initial concentration of Cr(VI) ion solution, time of contact, and weight of the polymer; investigated the effect of those factors and optimized them for maximum sorption efficiency. Also, the selective sorption of Cr(VI) ions from ternary solutions along with a competing metal ion species was investigated by the competitive adsorption method and found to be highly appealing for the selective adsorption-based removal of Cr(VI) ions from aqueous solutions.

Keywords: Chromium, ISNCPN, Selective Sorption

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Rauwolfia Serpentina Roots Derived Carbon Dots as a Fluorescent Sensor for the Detection of Mercuric Ions in Water

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ABSTRACT

This study uses a hydrothermal method to describe the facile, cost effective, and green synthesis of highly fluorescent carbon dots from the roots of the Rauwolfia serpentina plant. The produced carbon dots (CDs) have a size of 3.95nm and display good hydrophilicity and excellent photostability under various circumstances. Various analytical techniques are used to examine their properties. The fabricated CDs act as highly selective and sensitive fluorescent sensor for detecting Hg^{2+} ions in water. The fluorescent quenching mechanism is static and involves the interaction of surface functional groups of the CDs with the analyte. The LOD value obtained is in the nanomolar range, equal to 10.25 nM. The practical utility of the suggested sensor was established by real sample analysis with low relative standard deviation (RSD) values. Also, a minute concentration of the CDs shows excellent antifungal potency towards the fungal strain Aspergillus niger.

Keywords: Carbon dots, fluorescent sensor, fluorescent quenching, antifungal efficacy

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Facile Synthesis of Carbon Quantum Dots for The Selective Detection Of Levofloxacin

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ABSTRACT

Carbon dots(CDs) as a new type of carbon-based nanomaterial, have attracted broad research interest for years, because of their diverse physicochemical properties and favorable attributes like good biocompatibility, unique optical properties, low cost, abundant functional groups, high stability, and electron mobility. In the present work, we synthesized the carbon Quantum dots(CQDs) by hydrothermal method using thiourea and citric acid are used as a precursor for the preparation of the CQDs. Using a variety of analytical techniques, the optical and physical characteristics of as-synthesized CQDs were fully evaluated. The synthesized carbon dots are used to detect selectively by the levofloxacin drug. Carbon nanoparticles have a small size in the order of a few nanometres by all dimensions. Drugs are not good for our bodies so their detection is very essential. CDs have many properties these properties can easy to sense drugs and other materials. This sensor is very useful in the future.

Keywords: Sensing, CQD, drugs, levofloxacin, fluorescence enhancement

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Biosynthesis of silver nanoparticles using seeds of *Mangifera indica* and their characterization

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ABSTRACT

Biosynthesized nanoparticles are gaining popularity due to their distinctive biological applications as well as biologically active secondary metabolites from plants that aid in green synthesis. The aqueous seed extract of *Mangifera indica* (*M. indica*) was used in this study to easily create silver nanoparticles. The aqueous seed extract of *M. indica*, which served as a reducing and capping agent, was used to biosynthesize silver nanoparticles. Several methods, including UV-Visible specrtroscopy, scanning electron microscopy (SEM), Fourier transform infrared (FTIR) and energy-dispersive X-ray analysis (EDAX) were used to characterise the biosynthesized *M. indica* silver nanoparticles (Mi-AgNPs). The phytochemicals responsible for the capping and reduction of the biosynthesized Mi-AgNPs were identified through phytochemical analysis. The creation of AgNPs in the solution as a result of surface plasmon resonance (SPR) electrons on the nanoparticle surface is clearly indicated by the appearance of an absorbance peak at about 420 nm. SEM was analaysed that the prepared Mi-AgNPs had polymorphism forms. The reduction, capping, and stabilisation of the produced nanoparticles resulted in substantial and small changes of the peaks in the FTIR spectra of the M. indica seed extract corresponding to Mi-AgNPs. The silver element was responsible for the prominent peak at 3 keV in the EDX spectrum. The use of M. indica in the synthesis of AgNPs offers a number of benefits, including a process that is economical, effective, and environmentally friendly. It is also energy- and cost-effective, promotes healthier workplaces and communities, safeguards the environment, and results in less waste and safer products. For a wide range of biomedical applications, the potentially active phytoconstituents used in the plant-mediated production of nanoparticles are biocompatible.

Keywords: *Mangifera indica*, Silver nanoparticles, Seed extract, Phytochemical study, Biosynthesis.

Biomass Derived Carbon Dot-Based Nanosensors for Pollutant Detection

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ABSTRACT

Hazardous materials like insecticides, pesticides, fungicides, explosives, etc., cause severe environmental pollution, and the release of these into the environment should be managed effectively. As a unique type of zero-dimensional carbon nanomaterial, fluorescent carbon dots (CDs) have gained much scientific attraction in recent years [1]. Their exceptional properties, such as low toxicity, high photo, and chemical stability, robust chemical inertness, tremendous water solubility, and ease of functionalization, make them the best candidates for their use in a variety of fields including contaminants sensing [2]. Due to its advantages over chemical synthesis in terms of cost, environmental friendliness, repeatability, and simplicity, the green synthesis of CDs from natural carbon precursors has gained importance [3]. This work describes a straightforward fluorescence-based method using carbon dots (CDs) with a green chemistry synthesis process for the detection of the hazardous compound trinitrophenol (TNP). The blue fluorescent CDs with an average size of 2.86 nm were synthesized via the hydrothermal method from green sources. The fluorescence response of CDs showed a linear response with TNP. The limit of detection was determined to be 23.00 nM. The practical utility of the sensor was explored via real sample analysis. The findings of this work lead to the creation of a novel sensing system that can serve as a foundation for the design of sensing probes for the detection of hazardous substances.

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Optimized Biodiesel Production from Hibiscus Cannabinus seed oil using Barium Oxide (BaO) Nano-catalyst

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ABSTRACT

Biodiesel production from Hibiscus cannabinus seed oil provides an alternative energy means of producing liquid fuels from biomass for various uses. Biodiesel production by bio-oil and methanol in the presence of Barium oxide (BaO) nano-catalyst offers several benefits such as environmental, waste management and economically. A nano-catalyst of BaO was synthesized by thermal-decomposition method and calcinated at 450 °C followed by characterization using SEM, TGA, XRD, and FTIR techniques. The maximum conversion of Bio-oil to biodiesel was estimated to be 94%, at optimized experimental conditions, 60 °C, and 1:10 Bio-oil oil to methanol ratio, 1.5% by weight of catalyst loading rate and 110 minutes reaction time, which is among few maximum conversions resulted so far. Biodiesel parameter were analysised according to the American (ASTM D6571) fuel standards. All reactions are carried-out under atmospheric pressure and 1450 rpm of agitation.

Keywords: Biodiesel; BaO Nano- catalyst; Thermal- decomposition.

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Microwave-assisted Synthesis of Nitrogen-doped Carbon Quantum Dots as a Fluorescent Sensor for Amoxicillin

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ABSTRACT

A simple and facile fluorescence sensor for Amoxicillin detection was developed using nitrogen doped carbon quantum dots (N-CQDs) from a mixture of β-cyclodextrin and EDTA following a microwave irradiation method. Spectroscopic techniques such as UV-vis, PL, FT-IR, XRD, DLS, zeta potential, and TEM analyses were used to characterize the optical, chemical, and morphological properties of the system. The N-CQDs exhibited a blue fluorescence at 445 nm when exciting at 360 nm with a quantum yield (QY) of 15%. The N-CQDs are spherical in shape and have an average diameter of 6 nm. Amoxicillin is a commonly used antibiotic in human medicine. However, widespread distribution and overuse of Amoxicillin can pose environmental and health risks. The developed sensor demonstrates excellent selectivity and sensitivity with the linear range of 0-25 μM and detection limit of 80 nM. The quenching mechanism includes a combination of the stated quenching and the inner filter effect (IFE). The fluorescent approach was effectively applied for ultrasensitive detection of Amoxicillin in drinking water with satisfied recovery from 98.5% to 101.4%.

Structural and Spectroscopic Studies on Copper Complexes of N-bidentate Ligand: Biomimetic approach

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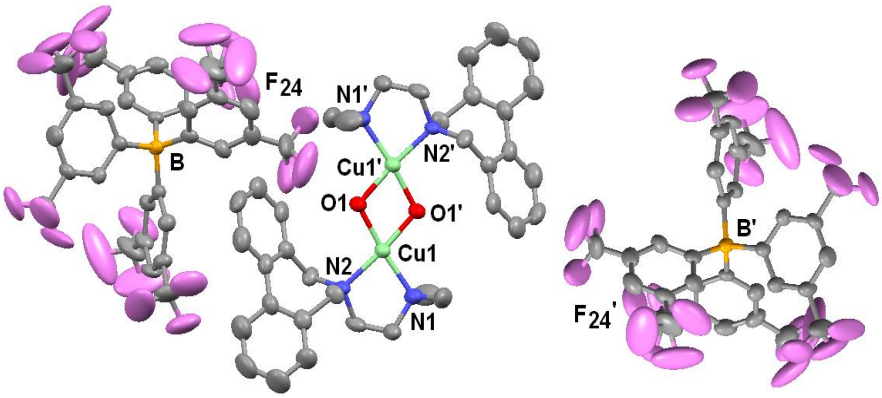
ABSTRACT

Structural, spectroscopic and reactivity studies on metal-dioxygen species is an active area of investigation, widely as models for metalloenzymes and natural copper proteins and to develop oxidation catalysts. Multidentate donor ligands have played key roles in such studies. Analogous study with bidentate ligands is limited [1,2,3]. We have employed a novel N-bidentate ligand, (N,N-bis((2,2'-methylene-1,1'-biphenyl)-N,N-dimethyl-ethylenediamine) (**L**) and prepared its copper(I) complexes and explored their reactivity with O_2. X-ray crystal structure analysis of novel dinuclear copper(II)-hydroxo complexes, $[Cu_2\mathbf{L}_2(OH)_2(ClO_4)_2]$ (**1**), $[Cu_2\mathbf{L}_2(OH)_2(NO_3)_2]$ (**2**) and $[Cu_2\mathbf{L}_2(OH)_2](BAr'_4)_2$ (**3**, Figure), their unusual spectroscopic properties using a combination of techniques and a preliminary reactivity study with t-BuOOH to form a Cu(II)-alkylhydroperoxo intermediate, and with bis(p-nitrophenyl)phosphate (BNPP) leading to P-O bond cleavage will be highlighted.



X-ray structure of $[Cu_2\mathbf{L}_2(OH)_2](BAr'_4)_2$

Keywords: bidentate ligands; metalloenzymes

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Single crystalline Au Nano and Microplates: Growth, Functionalization and tuning of Work Function

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ABSTRACT

Two-dimensional (2D) monocrystalline Au microplate draws significant interest due to its significance toward the future progress of optical nanocircuitry for high-speed communication and quantum computation applications. In this work, 2D Au microplates were synthesized by seedless aniline assisted polyol reduction with anisotropic control of the in-situ polyaniline oxidation states. Three different polyaniline oxidation states were identified by a novel algorithm based on subtraction deconvolution of UV-vis spectra: A (372 nm), B (680 nm), and C (530 nm). Time-dependent UV-Vis Spectra and SEM images of Au nanostructures showed that PAOS controls the 2D microplates shape, size, and crystallization parameters. Different growth parts related with relevant growth mechanism (protonation, deprotonation and thermal decomposition) were resolved. We found that state A is responsible for the nucleation of gold from the $AuCl_4^-$ solution (region i), state B is responsible for the aggregation of the nucleation sites (region ii), and state C is responsible for the 2D shape of the microplate and for the control of Au monocrystalline flake growth (region iii). We used a time-resolved deconvolution model for the solution-growth of nanomaterials, which is accurately describe the charge transitions (intra and inter transitions) and growth regimes by effective permittivity parameter in solutions. The work function of synthesized Au microplates altered with substituted benzene thiols. The photoelectron yield spectra (PYS) of benzene thiols functionalized Au microplates showed work function shift between 4.2 eV to 5.4 eV depending on the substituted benzene thiol. The results provide basic understanding of PAOS, and Au flake formation and functionalization, which influencing other anisotropic metals syntheses and functionalization with desired properties and monocrystalline nature for optoelectronic applications.

Plasmon and Upconversion enhanced Photocatalytic Activity of $NaGdF_4$:Yb:Er/Ag/TiO_2 under UV-Visible and near-infra red irradiation

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ABSTRACT

Environmental pollution has always been an important problem for the world and the severity of the pollution are increasing over the years. Pollutants, mainly organic dyes are responsible for water pollution. Photocatalysis is of the most efficient ways to decay organic pollutant into harmless CO_2 and water using vast abundant solar energy. Rapid recombination of the electron-hole pair and lack of visible light photocatalytic activity of TiO_2 limit the effective solar energy harvesting. A complete range of solar energy harvesting is essential for the enhanced photocatalytic activity and better usage of sunlight. A novel UV, visible and NIR active $NaGdF_4$:Yb:Er/Ag/TiO_2 catalyst was synthesized by oleyl amine assisted thermal decomposition method. The $NaGdF_4$:Yb:Er/Ag/TiO_2 was well characterized by XRD and TEM analysis to study the crystal phases and morphology images of the composite nanostructures. The synthesized $NaGdF_4$:Yb:Er/Ag/TiO_2 exhibited hexagonal crystal phase of $NaGdF_4$, face-centered cubic phase of silver and anatase phase of TiO_2. TEM elemental mapping of Ag and Gd show the silver and $NaGdF_4$ particles were in the range of 8-20 nm. The Ag and $NaGdF_4$ particles were completely covered by TiO_2 particles and the composite particles were in the range of 100 – 500 nm. The composite particle showed UV-visible absorption up to 750 nm. $NaGdF_4$ upconversion luminescene spectrum showed four peaks at 523, 542, 656 and ~ 800 nm under 980 NIR laser irradiation. The intensity and ratio of the peaks were reduced when adding Ag and TiO_2 particles. The luminescent intensity changes confirmed the energy transfer (NIR to visible) among $NaGdF_4$:Yb:Er, Ag, and TiO_2 particles. The optical property of the $NaGdF_4$:Yb:Er/Ag/TiO_2 confirmed that the catalyst may well absorb UV, visible and NIR light energies. The UV-visible and NIR active photocatalytic ability of the $NaGdF_4$:Yb:Er/Ag/TiO_2 catalyst was tested by Rhodamine B dye degradation studies. The catalyst exhibited photocatalytic activity under both the UV-Visible and NIR irradiations. The photocatalytic results confirmed that the energy transfer among $NaGdF_4$:Yb:Er, Ag, and TiO_2 particles drove the NIR driven photocatalytic activity of the catalyst. Therefore, the $NaGdF_4$:Yb:Er/Ag/TiO_2 catalyst generated the electron-hole pair upon NIR illumination, which is responsible for the photodegradation. The study established a synthesis of novel UV, visible and NIR-responsive $NaGdF_4$:Yb:Er/Ag/TiO_2 photocatalyst and the energy transfer and photocataytic mechanism among $NaGdF_4$, Ag and TiO_2 particles.

Peramivir: Degradation and Identification of Impurities and the Endorsement of HPLC Method

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ABSTRACT

Background: Peramivir, a neuraminidase inhibitor that acts as a transition-state analogue for influenza, preventing new viruses from emerging in infected cells, has also been approved for the intravenous administration.

Objective: To validate the HPLC method to identify the degraded products of the antiviral drug Peramivir.

Methods: Herein, we report the identification of degraded compounds formed after the degradation of the Peramvir an antiviral drug done by the acid, alkali, peroxide, thermal and photolytic degradation. Peramivir separation and quantification at the toxicology level, concern method was developed.

Results: A sensitive and reliable liquid chromatography-tandem mass spectrometry method for the quantitative analysis of Peramivir and its contaminants was developed and validated in accordance with ICH guidelines.The proposed protocol was in the 50-750 g/mL range. RSD values less than 2.0% indicate good recovery in the range of 98.36%-102.57%. Within the studied range, the calibration curves demonstrated good linearity, and the correlation coefficient of fitting exceeded 0.999 for each impurity. Contaminant quantitative analysis revealed the high efficiency at a low level.

Conclusion: Given its ability to separate degradation products, quantitative analysis is used to detect and quantify known and unknown impurities and degradants in the Peramivir drug substance during routine analysis and stability studies. No significant degradation was found in peroxide and photolytic degradation studies.

A Robust RP-HPLC method for the determination of Relugolix's related substances and characterization of its degradant using LC-MS/MS

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ABSTRACT

Background: Relugolix, an anticancer medication, helped treat prostate cancer. Consumed title compound undergo degradation and results in the side effects of the patients. The degraded compounds may the responsible for the side effects. Henceforth, it is mandatory to identify the degraded compounds.

Objective: To validate the HPLC method to identify the degraded products of the anticancer drug Peramivir.

Method: Herein, we report the identification of degraded compounds formed after the degradation of the Relugolix an anticancer drug done by the acid, alkali, peroxide, thermal and photolytic degradation. Peramivir separation and quantification at the toxicology level, concern method was developed.

Results: All contaminants, as well as Relugolix, had LOD and LOQ determined based on the concentration of the test substance. Studies on recovery were successful, and a correlation coefficient of 0.999 for Relugolix and related compounds indicated that the approach is linear within the parameters it was designed.

Synthesis of Spherical $CaWO_4$ Microsphere: Synthesis, Luminescence and Catalytic Property

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ABSTRACT

Surfactant-free and various surfactants assisted Scheelite type calcium tungstate ($CaWO_4$) were prepared via a simplistic co-precipitation technique. The crystal system of the prepared $CaWO_4$ materials was authenticated by powder X-ray diffraction (PXRD) and the Rietveld profile refinement technique. The micrographs of the surfaces and elemental composition of the $CaWO_4$ materials were investigated using scanning electron microscopic (SEM), transmission electron microscopy (TEM), and energy dispersive spectroscopy (EDS) measurements, respectively. Interestingly, the surfactant CTAB assisted $CaWO_4$ material has been emitted intense light green emission at the wavelength at around 500 nm due to the WO_4^{2-} luminescence center. Moreover, the prepared $CaWO_4$ materials have been dramatically degraded to an organic dye methylene blue under solar irradiation. Compared to other host and surfactant-loaded catalysts, the CTAB loaded $CaWO_4$ revealed the soundest-diligent catalyst towards the natural sunlight relieved degradation of dye with 40 min.

Improved photocatalytic capability of pebble stone like $CuMoO_4$ photocatalyst for the eradication of organic pollutant

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ABSTRACT

In this study, a facile hydrothermal process was used to fabricate the $CuMoO_4$ nanomaterial. $CuMoO_4$ nanoparticles were used to study the photocatalytic efficiency of methylene blue (MB) in aqueous phase while it was illuminated by visible light. To explore the nanoparticles' structure, size distribution, and qualitative elemental analysis of their composition, the produced nanoparticles were characterized using XRD, FT-IR, SEM, UV-vis diffuse reflectance spectra, and EDAX spectroscopy. Under visible light, the CuMoO4 nanomaterial had a greater rate of MB dye degradation. $CuMoO_4$ catalyst was used to optimize the photo degradation process at a concentration of 1 μM (30 mg). At 50 minutes, a maximal photocatalytic performance of 94.7% was attained. In-depth research has been done on factors influencing the photocatalytic process, such as adsorbent dose, concentration of the catalyst and scavengers, recycling efficiency, and MB concentration.

Keywords: $CuMoO_4$; Visible light; Methylene blue; Photodegradation; Efficiency

GCN Decorated Manganese Oxide for Photocatalytic Degradation of Methylene Blue

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ABSTRACT

We have synthesized different concentrations of graphitic carbon nitride (GCN) (20%, 40%, 60%, and 80%) decorated manganese oxide (Mn2O3) for photocatalytic degradation of the organic contaminant methylene blue (MB) in the current study. Powder X-ray diffraction (PXRD) research was used to investigate the crystalline nature of synthesized GCN-coated Mn2O3. Scanning electron microscopy (SEM) analysis was used to investigate the surface morphology of produced materials. The element purity of GCN-adorned Mn_2O_3 materials was studied by energy dispersive spectroscopy (EDS) to identify the composition of elements. Fourier transformation infrared (FTIR) spectroscopy was used to investigate the functional group analysis of synthesised GCN adorned Mn2O3. GCN adorned Mn2O3 materials with different concentrations of GCN (20%, 40%, 60%, and 80%) were used as photocatalysts for the degradation of MB dye. Under visible light illumination, 60% of GCN decorated Mn2O3 demonstrated excellent photocatalytic performance for MB breakdown, with a capability of above 99%. When compared to other Mn2O3 materials, the improved photocatalytic activity was attributed to the good crystallinity, defined shape, superior optical band gap, and smaller particle size.

Keywords: Mn_2O_3, PXRD, FT-IR, Methylene Blue, Degradation

Antimicrobial Activities and Catalytic Oxidation of Alcohols by Ni(II) Schiff Base Complexes

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ABSTRACT

Air stable Ni(II) Schiff base complexes *viz.* [Ni(L^1)(PPh_3)] and [Ni(L^2)(PPh_3)] [where L^1 and L^2 are dianions of Schiff base ligands, respectively] have been synthesized and characterized by analytical and spectral (electronic, FT-IR, ^1H, ^{13}C and ^{31}P NMR) methods. The assignment of all the aromatic carbon-hydrogen resonances is made on the basis of ^1H-^{13}C HSQC spectrum of the complexes. The Schiff base ligands behave as a bibasic tridentate ligands and bonded through ONO and ONS mode. A square planar structure has been proposed on the basis of spectral data. Novel Ni(II) Schiff base complexes exhibited good antimicrobial activity towards the strains *Staphylococcus epidermidis* and *Escherichia coli*. Thermal and air stability of the complexes offer the advantage of oxidation of alcohols.

Keywords: Nickel(II), Schiff base complexes, Square planar nickel, Tridentate ligands, Oxidation of alcohols.

SYNTHESIS, SPECTRAL INVESTIGATION AND ELECTROACTIVITY OF Ni(II) SCHIFF BASE COMPLEXES

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ABSTRACT

New four coordinated Ni(III) complexes have been synthesized using Schiff bases formed by condensing actetoacetanilide/acetoacetotoludide with o-aminophenol/ o-aminothiophenol in 1:2 stoichiometric ratio. The new complexes have been characterized by analytical and spectral (IR, electronic, and NMR) studies. An octahedral structure has been proposed for all the complexes. All complexes show good catalytic and antimicrobial activities. The Schiff-base complexes show better activity in catalysis. The synthesized nickel(II) Schiff base complexes were electrochemically sensitive towards the detection of nicotine even at micromolar concentrations.

Structural analysis of surprisingly formed Cu(II) cubane through the specific cleavage of >C=N- and >C=S- of a Schiff base ligand and its biological activities

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ABSTRACT

Extraordinary specific breaking of the carbon-sulfur linkage of the thiosemicarbazone moiety from a Schiff base has been watched the blue, bringing about the development of a four coordinated tetra Cu^{II} cubane containing triphenyl phosphine and μ_3-S as ligands. At the same time, the ketimine group of the Schiff base ligands also got ruptured to regenerate the diketone used for the synthesis of thiosemicarbazone ligand. The synthesized complex was spectrally and structurally investigated. The crystallographic information reveals that the complex is having the shape of a cubane, whereas the alternate four corners were occupied by tricoordinated copper and the other corners are by μ_3-S respectively. μ_3-S behaves as a ligand which is having the binegative site and neutral site to get bonded with the copper as bridging ligand. Antimicrobial and antioxidant efficacy were explored and shows a better results than the controls used.

Keywords: Carbon-sulfur, Cu^{II} cubane, μ_3-S Thiosemicarbazone Antimicrobial Antioxidant

Anticorrosion Activity of Bioemulsions on Metal-Environment Interface

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ABSTRACT

The influence of Ricinus communis oil on electrochemical corrosion of steel in oil-in-water emulsions under controlled hydrodynamic condition was investigated. Emulsions from renewable biobased sources have gained prominent role in food and pharmaceutical industries as green excipients. The emulsion system under study was prepared from ricinus communis oil, hexadecyl polyglucoside and brine solution in which ricinus communis oil constitute the non-polar phase and surfactant constitute polar phase. The efficiency and effectiveness of these emulsion system highly influenced by their constituents and composition. Thus the stability of the as-prepared emulsion is analyzed through the optimization of various emulsion formulation factors such as viscosity, and creaming rate. The stability of emulsion was observed to increase with viscosity since it makes the particles to distribute evenly. The application of the emulsion on metallic surface under controlled hydrodynamic conditions was studied using potentiodynamic polarization Tafal plots. The newly formulated emulsion showed corrosion inhibition on the tested alloy steel and their corrosion rate was reduced to 0.5598 mm/year. The antimicrobial activity of this versatile emulsion was also assessed using in-vitro assay. This emulsion formulation can be used economically in industrial application as it may reduce the preventive maintenance, replacement of corroded equipment and contamination of product.

Keywords: Ricinoleic acid: corrosion potential: oil-in-water emulsion: Corrosion inhibition

Synthesis and characterizations of nano Sand filled Unsaturated Polyester Resin

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ABSTRACT

Lightweight materials are a new class of engineering materials with excellent mechanical properties that lead to a wide array of possibilities for oil/seawater application. Unsaturated polyester resin (USPER), a thermosetic material produced positive signal towards the same. In this work, nano Sand filled USPER nanocomposite was prepared by free radical curing mechanism. The resultant polymer/nanocomposite was characterized by DSC, TGA, WCA, SEM, FESEM, color mapping, TEM and EDX. The prepared composite was tested for tensile strength, elongation, compression, impact, flectural modulus, dielectric strength, arc resistance, water absorption, hardness and thermal aging measurements. The mechanical testing confirmed that while increasing the % of nano Sand, the mechanical properties were increased accordingly. The 2.5% nano Sand based USPER exhibited the highest mechanical properties. The flectural modulus of nano Sand filled USPER was increased by 1158 %. The final composite exhibited hydrophobic character (103^{o}). The water flux and % oil rejection of the membranes were tested. The results are carefully analyzed and compared with the literature reports.

Mechanical and physico-chemical characterizations of Eggshell reinforced and nano Sand filled Unsaturated Polyester Resin

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ABSTRACT

A light weight and non-corrosive unsaturated polyester resin (USPER) with improved mechanical properties was synthesized in the presence of methylethylketone peroxide at room temperature with the aid of egg shell (ES) as a reinforcing agent and nano Sand as a typical filler. The prepared USPER/nanocomposite was tested by various mechanical and thermal instruments. The experimental results showed that while increasing the % of nano Sand the mechanical properties were increased proportionally. The SEM image showed the presence of voids on the surface of USPER. The EDX spectrum showed the presence of Alumina and silica nanoparticles. Efficiency of oil/seawater separation was determined using USPER nanocomposite membrane.

Non-Isothermal Degradation kinetics of Poly(anthranilicacid)/Sand nanocomposites

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ABSTRACT

Peroxydisulphate (PDS) initiated chemical polymerization of anthranilicacid (AnA) was done under nitrogen atmosphere at 0-5 ^{o}C with vigorous stirring both in the presence and absence of Sand using Rosebengal (RB) as an end capping agent. The prepared polymer and its nanocomposite was analyzed by UV-visible, TGA, DSC, SEM, EDX, FTIR, CV, FES, HRTEM and XRD instruments. The thermal stability of the prepared polymers was tested through non-isothermal degradation kinetics. Further, the thermodynamic parameter values were determined. The 3% weight Sand loaded poly(anthranillicacid) (PAnA) system showed the % yield of 90.3% with the conductivity value of 4.31×10^{-2} S/cm. The added Sand accelerated the rate of polymerization (Rp). The photo-conversion efficiency of PAnA/Sand nanocomposite system is higher (1.49%) than the RB end capped PAnA system. The experimental results are thoroughly analyzed and compared with literature values.

Synthesis and characterizations of PVC-g-PSF membrane via Friedel-Crafts alkylation reaction

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ABSTRACT

Since the last decade, application of forward osmosis (FO) has been expanded to purify wastewater or to supply fresh water resources, including seawater desalination, oil and gas remediation, osmotic membrane bioreactors, concentrating underground brine, sludge dewatering, and industrial water recycling. The crucial challenges related to the application of FO are draw solute (DS) development and FO membrane fabrication. In order to solve this problem, in the present research work polysulfone (PSF) was chemically grafted onto poly(vinylchloride) (PVC) backbone via Friedel-Crafts alkylation reaction at 85^{o}C under nitrogen atmosphere with vigorous stirring for 4 hours. The resultant product was characterized by FTIR spectroscopy, ^{1}H-NMR spectroscopy, DSC, TGA, Water contact angle measurement, SEM and EDX like analytical tools. Phase inversion methodology was adopted for the fabrication of membrane towards the filtration of dye effluents.

Synthesis and characterizations of fluorescent diblock copolymer via ring opening polymerization

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ABSTRACT

The ring opening polymerization (ROP) of tetrahydrofuran (THF) and ε-caprolactone (CL) was carried out at 160 °C for 2 h under N_2 atmosphere using two different fluorescent dyes called fluorescein (Flur) and rhodamin6G (R6G) as a novel initiator in the presence of stannous octoate as a catalyst. The structure of the dye centered diblock copolymer synthesized was confirmed by ^{1}H-NMR spectra. The melt transition temperature and thermal stability of the diblock polymers were determined by DSC and TGA respectively. The FT-IR spectra indicated the functional groups present in the dye grafted homopolymer and diblock copolymers. The increase in molecular weight (*M*w) of the dye centered diblock copolymer was confirmed by the GPC measurement. The conjugation of dye with the polymer backbone was carried out by a single step method without using any hazardous solvents is the novelty of the present research work.

SYNTHESIS AND STUDIES OF CONDUCTING MATERIALS BASED ON POLYANILINE-SILVER NANOCOMPOSITE

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ABSTRACT

In recent years, there has been growing interest in the development of conducting polymers (CPs) as prospective materials for technological applications. The electrical conductivity of the conducting polymer is due to the ordered conjugation with extended π-electrons. Both doped and dedoped Polyaniline-silver (PANI-Ag) nanocomposites were synthesized using chemical oxidative polymerization of aniline monomer in the presence of nitric acid and ammonium peroxydisulfate. The nanocomposites were characterized by UV-vis. spectroscopy, Fourier transform infrared (FT-IR) spectroscopy, X-beam diffraction (XRD), and Conductivity studies .The estimation of the optical band gap is found to diminish after doping. FT-IR and UV-visible spectroscopy show a significant shift in both the doped and dedoped PANI-Ag nanocomposites. D.C. conductivity of the composites was varied with temperature. PANI-Ag nanocomposite behaves as a semiconductor at low temperature and as a metal at high temperature.

Keywords: conducting polymers, nanocomposites, polyaniline.

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A short review on solid-state electrolytes for lithium-ion batteries

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ABSTRACT

A lithium-ion battery is a series thought in the current scenario. In this review article the different types of solid electrolytes such as Nasicon, Lasicon, Lipon, Garnet, and Perovskite structures are reviewed successfully the aim is to prepare the best solid electrolyte under good circumstances on battery cell preparation and conductivity.

Keywords: Lithium-ion battery, Type of Solid electrolytes.

Synthesis, Characterisation and Multitargeted biological applications of Novel Ruthenium(II) isatin based Schiff base complex

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ABSTRACT

The present study discloses the synthesis of novel Ru(II) isatin Schiff base complex cis-[Ru^{II} $(Phen)_2$ FPIMI] $ClO_4.2H_2O$(Formula 1) from the reactions between cis-[Ru $(Phen)_2$ Cl_2].$2H_2O$ and 4-fluoro phenyl imino methyl isatin(FPIMI). The new complex was characterized by elemental analysis and spectral(UV-vis, IR, ^1H NMR and EPR) methods. The redox properties are studied by cyclic voltammetry. Further the complex was subjected to the biological investigations such as DNA intercalation studies, anti bacterial, anti fungal, *in vitro* cytotoxic activities, antibacterial and anti osteoporotic studies. DNA intercalative assay was followed by UV-vis spectral titration & fluorescence spectroscopic studies with relatively high DNA binding constant, K_b=3.4±2 10^5 M^{-1} at room temperature. The above studies showed intercalative mode of cleavage with Calf Thymus(CT) DNA. The newly synthesized ruthenium(II) complex exhibited more effective with less systemic toxicity along with good inhibitory activity against osteoporosis. Its IC_{50} value observed as 22±0.5 μM. The compound is also showed excellent inhibition against bacteria and fungi. This compound is exhibiting multiple biological activity and hence multitargeted drug.

Key Words: Isatin Schiff base, Ruthenium(II) Complex, DNA Binding, Anticancer, Cytotoxic Evaluation, Tumor Cell Lines, Anti osteoporotic, Anti bacterial and Anti fungal

Cytotoxic evaluation of Ru(III) complexes; their DNA/BSA binding by *in vitro* and *in silico* approaches

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ABSTRACT

Herein, we report the synthesis and characterisation of a series of Ru(III) complexes. UV–Vis spectroscopic characterisation was supported by TD-DFT theoretical simulation using Gaussian software. Different reactivity parameters were calculated from the energy difference between HOMO and LUMO of the complexes by DFT. The Docking studies revealed that these complex binds in to the minor groove of the DNA and then bends in such a way that it follows the curvature of the DNA groove. The bonding mode of the labile ligands was confirmed by NBO analysis. Interaction of the complexes with DNA has been observed by gel electrophoresis experiment. DNA binding nature as well as binding constants of the complexes were measured with UV–Vis and fluorescence spectroscopic method. The binding nature of the complexes with DNA was confirmed by viscometric titration. Interaction of the complexes with BSA was investigated by UV–Vis and fluorescence titration method. *In vitro* anticancer activity has been screened for all the synthesised ruthenium(III) complexes on human breast carcinomas MCF-7 and MDA-MB-231 against the globally acknowledged anticancer drugs. Cell cycle progression has been analyzed with MCF-7 cell lines to observe the probable death mechanism, and toxicity of the complexes has been measured by ROS generation on MCF-7 cell lines. In summary, the above findings may provide useful information to assist in the design of new metal complexes having enhanced biological activity.

Keywords: Ruthenium(III) complexes, DNA & BSA binding, Anticancer activity, DFT calculations, ROS generation and Molecular modelling.

Anticorrosion performance of functionalized graphene oxide encapsulated epoxy nanocomposite coating on mild steel

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ABSTRACT

The functionalization of graphene oxide (GO) with many organic moieties and their dispersion in polymer play a vital role in the corrosion protection performance of nanocomposite coatings. In the present work, the functionalized GO (fGO) with 3-amino-1 2 4-triazole 5 thiol (ATT) has been synthesized and characterized by Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) studies. The corrosion protection evaluation of fGO grafted epoxy nanocomposite coatings on mild steel is investigated using elecrochemical impedance spectroscopy (EIS), Potentiodynamic polarization studies and scanning electrochemical microscopy (SECM). The analysis of EIS data revealed high film, charge transfer resistances and low capacitance for the fGO +epoxy coated mild steel. Potentiodynamic Polarization studies showed high corrosion potential (E_{corr}) and low corrosion current (I_{corr}) values for fGO +epoxy coated mild steel. SECM analysis showed less current distribution (0.5 I/nA to 2.3 I/nA) at the scratched surface of fGO grafted composite coatings compared to neat epoxy coatings(2A to 10A) on mild steel. The presence of sulphur and nitrogen present in the fGO facilitated the enhanced corrosion protection performance of mild steel. The surface morphological studies of fGO along with epoxy coatings were analyzed by field emission scanning electron microscopy (FE-SEM) with energy dispersive X-ray analysis (EDX). Mechanical properties of the coatings were also found to be improved in the presence of modified GO particles as evidenced by hardness test and pull off adhesion test.

Keywords: Graphene oxide; surface modification; anticorrosion; SECM; EIS

A comparative study on the electrochemical corrosion behavior of epoxy coated carbon steel and API X-56N pipeline steel in 3.5% NaCl solution

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ABSTRACT

Steel pipelines, buried under the soil and protected by the protective coatings, are used for oil and gas transportation. These pipelines are one of the critical infrastructures for energy transportation and therefore became lifelines of modern society. Protective coatings are used to enhance the corrosion resistance of buried pipelines. Electrochemical Impedance Spectroscopy (EIS), Potentiodynamic polarization and Scanning Electrochemical Microscopy (SECM) techniques were used to evaluate the corrosion protection performance of epoxy coated API X-56N pipeline steel and carbon steel with a scratch in 3.5 % NaCl solution at different immersion time. The increase in the charge transfer resistance and film resistance of the coated X-56N steel is due to the presence Mn and Si in the steel. SECM was measured that dissolution of Fe^{2+} was suppressed at the scratch on the coated X-56N steel due to the higher resistance for anodic dissolution of the substrate. It has been found that the coated carbon steel corrodes in the chloride solutions faster than the coated API X-56N 5L steel under the same conditions. Increasing the exposure period in the 3.5 wt % NaCl solution for the samples from 0 h to 20 h showed a significant reduction in the corrosion parameters for both carbon and X-56N steel. It was confirmed clearly that the coated X-56 N steel is superior to coated carbon steel against corrosion in sodium chloride solutions. SEM/EDX analysis showed that Mn and Si were enriched in corrosion products at a scratched area of the coated steel after corrosion testing. FIB-TEM analysis confirmed the presence of the nanoscale oxide layer of Mn and Si in the rust of the steel, which had a beneficial effect on the corrosion resistance of coated steel.

KEYWORDS: *SECM; EIS; polarization; Corrosion; pipeline steel; SEM/EDX*

Synthesis, Characterization of Palladium(II) Schiff Base Complexes: Catalytic Activity in the Suzuki Carbon-Carbon Coupling Reactions

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ABSTRACT

The reaction of tri dentate Schiff base ligands (HL_1-HL_4) and Ruphosh as co-ligand with $Pd(OAc)_2$ in 1:1 molar ratio in acetonitrile medium afforded a series of palladium(II) Schiff base complexes $[Pd(L_{1-4})_2]$ (**1**–**4**). All the palladium complexes are air stable and fully characterized by elemental analysis, FT-IR, UV-Vis and ^{1}H and ^{31}P-NMR spectral methods and single crystal XRD. Further, palladium-catalyzed protocol for Suzuki Carbon-Carbon coupling reactions by these complexes have been developed, enabling to obtain biaryl products in good yield.

Keywords: Palladium complexes; Schiff base; Characterization; Single crystal; Suzuki coupling.

Chromium induced visible light absorption in $Zn_{0.98}Cu_{0.02}O$ and visible light driven photocatalytic activity

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ABSTRACT

Chromium doped $Zn_{0.98}Cu_{0.02}O$ ($0 \leq x \leq 0.02$) nanoparticles were successfully synthesized via co-precipitation method. They had been characterized by using x-ray diffraction (XRD), Energy dispersion X-ray (EDX), scanning electron microscopy (SEM) and UV-Visible absorption spectra. XRD pattern revealed that the samples possess hexagonal wurtzite structure of ZnO without any secondary phase after copper and chromium co-doping. Optical absorption analysis of the samples showed a red shift in absorption band edge. The band gap energy of the nanoparticles had been decreased from 3.78 eV (Cr = 0%) to 3.65 eV (Cr = 2%) by chromium doping and their possible mechanism have also been discussed. The synthesized NPs had better photodegradation efficiency against Methylene blue (MB) dye. The visible light absorption induced by the Cr dopant enhanced the photocatalytic efficiency of Cu and Cr co-doped ZnO NPs under visible light irradiation.

Keywords: ZnO Nanoparticles, X-ray diffraction, Optical properties, Co-precipitation, Methylene blue.

Functional, Structural and Antimicrobial analysis of Strontium Oxide nanoparticles through *Solanum virginianum* plant extract

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ABSTRACT

Even now in richer countries, food loss and waste due to microbial protein degradation still affect all varieties of foods on a global scale. According to estimates, up to 40% of the world's food is lost each year owing to a variety of issues, such as microbial deterioration [1]. Currently looking for safe and alternative antimicrobial agents to overcome this type of activity, the advent of nanotechnology has given rise to the possibility of combating deadly microorganism [2]. Among the Metal oxide, the structural diversity and wide range of applications of strontium oxide make it significant. It functions similarly to calcium in humans, aiding in bone growth and Osseo integration. In the present research work, Strontium Oxide nanoparticles (SrONPs) were synthesised by using *Solanum virginianum* plant extract. The synthesized nanoparticles were analysed by Fourier Transform Infrared spectroscopy (FTIR), X-ray diffraction analysis (XRD), UV-Vis absorption spectra, Scanning electron Microscope (SEM), and Antimicrobial analysis. The presence of C-O, O-H, C-C, and C-N peaks indicates that SrONPs are prepared using the *Solanum virginianum* leaf extract as reducing agent and also acting as capping agent on the surface of metal oxide nanoparticles. XRD and SEM study showed that the SrONPs had spherical shape and the average particle size was about 80 nm. The UV-Vis spectroscopy showed two transmittance peaks around 270 nm and 330 nm, indicating that the SrO NPs are pure. The antimicrobial efficiency of SrONPs was tested against the growth of *bacterial* and *fungal* species using disc diffusion method. The obtained results of clear zone inhibition values (mm) indicate that the test samples were exhibited significant antimicrobial activity compared to *Tetracycline* and *Flucanazole* standard drugs. **It is concluded that the intense Antimicrobial activities analysis of prepared** SrONPs **were addressed in the food packaging Industry.**

Keywords:
Strontium Oxide nanoparticles, *Solanum virginianum* and **food packaging Industry**.

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Chromene Carbohydrazide- Schiff Base as a turn-off chemosensor for In^{3+} ion and its application to DrG cell imaging

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ABSTRACT

A new 7-(diethylamino)-2-oxo-2H-chromene-3-carbohydrazide design to synthesize a Schiff-based ligand for the selective detection of cations The Schiff base ligand **L** was synthesized for the selective recognition of In^{3+} ions in DMSO:H_2O (7:3, pH = 7.4). Probe **L** exhibits a selective turn-off fluorescence response at 488 nm with In^{3+} ions. By Job's plot and ESI mass analysis, the probe **L** forms a 1:2 stoichiometry complex with an estimated association constant of 4.75×10^4 M^{-2} with In^{3+} ions. Metal induces CHEQ (chelation-caused fluorescence quenching) to reduce the intensity of the probe **L**'s emission. The limit of detection was found to be 4.3 nM; the time response of the sensor is instantaneous; and its reversible nature was confirmed using EDTA additions. For on-site applications, solid substrates (test-strips) were designed and tested for fast, reliable, user-friendly, and real-time sensing of In^{3+} ions. The binding mechanism of probe **L** with In^{3+} ions was investigated using ^1H NMR titration and DFT/TD-DFT studies. Furthermore, we investigated the real-time applicability of Probe **L** in DrG cell lines for live cell imaging applications.

Keywords: Chemosensor; Carbohydrazide; Aluminum; Indium; Cell Imaging; DFT

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A comprehensive review on the plant mediated synthesis of selenium nanoparticles and its biomedical applications

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ABSTRACT

While numerous nanoparticles are emerging recently, selenium-based nanoparticles have a unique advantage towards human health as they have low toxicity and greater compatibility with human organs and tissues. Also, it forms an essential micronutrient and plays a key role in boosting the body's immune system. Hence, they are mainly used for biomedical and pharmaceutical applications. Studies were carried out pertaining to the applications of selenium nanoparticles in therapeutics of tumour cells, microbes, pathogens, viral-based infections, diabetes and other antioxidant-related applications. Besides, certain ligands are combined with selenium nanoparticles to achieve targeted drug delivery. Plant-mediated synthesis has gained importance when selenium nanoparticles are synthesised by physical, chemical, and other methods as they are biocompatible and environmentally friendly. Further, plants are comprised of alkaloids, phenols, proteins and flavonoids, which form the major part of raw material as reducing agents for the synthesis as well as stabilisation of selenium nanoparticles. Overall, this review showcases the individual plants utilised for the production of selenium nanoparticles along with their fabrications with other nanoparticles to form nanocomposites. This review also demonstrates the characterisation of selenium-based nanoparticles using Ultraviolet–Visible spectroscopy, transmission electron microscopy, Raman spectroscopy, scanning electron microscopy and other related techniques. Finally, their applications in the biomedical field, such as therapeutics towards fungal and other microbial infections, cancer, and their anti-inflammatory properties are discussed.

Keywords: Selenium, drug delivery, cancer cells, phytochemicals, diabetes, anti-inflammation

GREEN SYNTHESIS AND CHARACTERIZATION OF ZINC OXIDE NANOPARTICLE FOR PHOTOCATALYTIC DEGRADATION

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ABSTRACT

One of the most important challenges for chemical researchers is the development of advanced green chemical technologies and processes in organic synthesis and environmental conversions. Many traditional catalytic processes for chemical production use toxic and hazardous substances as catalysts or solvents, making them unsustainable in terms of resources, environmental impact, and energy efficiency. The main reason that Photocatalysis is sustainable from a catalytic standpoint is the photonic activation mode of the photocatalyst rather than the thermal activation mode typical of traditional industrial processes.

ZnO nanoparticles were prepared using ultrasonic assisted co-precipitation process. The process of the solution greatly improves the nucleation process and homogeneity of the nanoparticles. Similar procedure was used to prepare leaf extract with ZnO nanoparticles. The prepared powders were characterized using XRD, FTIR, UV-Vis technique. The degradation percentage of dyes in waste water improved with increasing intensity of Photocatalysis using suspended particles to remove contaminants in aqueous systems is an efficient process, but the subsequent removal of the particles from the systems adds extra process steps. In this regard, use of supports for the catalysts is found to be helpful. However, there is an inverse relationship between the adhesion of a catalyst to a support and its photocatalytic activity.

Keywords: ZnO Nanoparticles, Co-precipitation, Photocatalyst, Degradation and Spectral Analysis

Palladium(II) Complexes Containing Tridentate Schiff base Ligands and Pyridine: Synthesis, Characterization, DFT study and Catalytic activity in the Sonogashira Coupling Reactions

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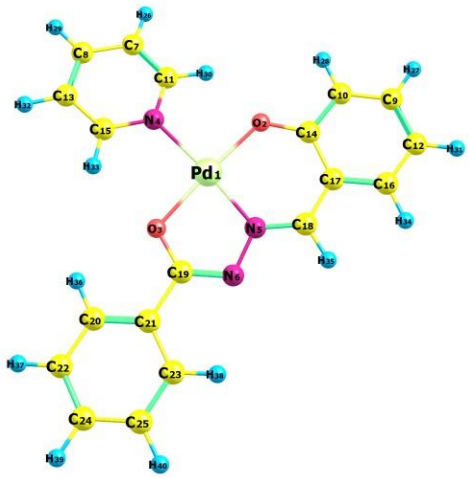
ABSTRACT

A new class of palladium(II) complexes of the general formula [Pd($L_{1–4}$)(Py)] (**1–4**) bearing benzoylhydrazone based Schiff base ligands have been synthesized. The synthesized complexes were characterized by elemental analysis, spectroscopic (FT-IR, UV-Vis and ^{1}H-NMR) and DFT studies. Theoretical computations using density functional theory (DFT) studies on these new complexes confirm their distorted square-planar geometry and their stability. Further, these complexes show good catalytic activity in the Sonogashira coupling reactions of aryl halides and phenylacetylene in ethanol media to afford the corresponding C-C coupling products in high yields.



DFT optimized geometry of the complex 1 showing distorted square planar arrangement

Keywords: Palladium(II) complexes; Schiff base; DFT; Sonogashira coupling.

Gold Catalyzed Mechanosynthesis of Triazolyl-*bis*(indolyl)methane Pharmacophores: A Prelude to Molecular Electronic Properties and Biological Potency

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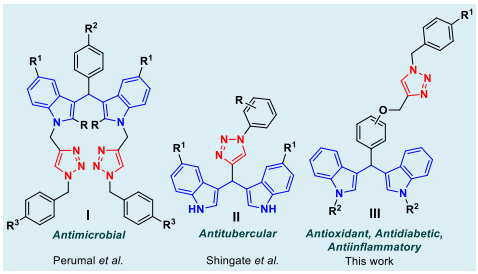
ABSTRACT

Due to their well-established biological efficacies, chemical compounds with both 1,2,3-triazole and bis(indolyl)methane units have attracted a lot of interest in medicinal chemistry.However, triazoles linked at the bridging position of *bis*(indolyl)methane is a logical and unexplored design approach. In this regard, nine new triazolyl-*bis*(indolyl)methane conjugates under gold catalyzed ball-milling conditions were accomplished. Comparative evaluation on absorptive and emissive properties of the synthesized dyads were also analyzed. To unravel the influence of different peripheral substituents on the electronic structure and π-orbital properties, DFT calculations were performed. Screening of molecules for free radical scavenging, anti-inflammatory and antidiabetic showed comparable potency against reference drugs. In particular, three Triazolyl-bis(indolyl)methane compounds displayed good efficiency of α-amylase inhibition. The DNA gyrase inhibitory potential of all compounds were assessed *in silico* which revealed high binding affinity (ΔG = −8.99 Kcal/mol) for 3,3'-((4-((1-(4-chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)methylene)bis(1H-indole) followed by 3,3'-((4-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)phenyl)methylene)bis(1H-indole) (ΔG = −7.80 Kcal/mol) with the targeted protein.



Keywords: Triazolyl-bis(indolyl)methanes • mechanosynthesis • π-orbital properties • biological screening • molecular docking

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An interpretation of the functional behaviour of lithium orthosilcate doped with Yttrium ($Li_4Y_{0.02}Si_{1-0.75(0.02)}O_4$)

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ABSTRACT

The solid-state electrolytes with high energy density could be used with lithium-ion batteries to increase operational safety. The solid electrolyte made of lithium superionic conductor (LISICON) is used for lithium-ion mobility. In this study, yttrium oxide (Y_2O_3) is used as a dopant added to the inorganic solid electrolyte of lithium orthosilicate (Li_4SiO_4) carried out the synthesis in solid-state route. The resultant powdered samples are analysed using XRD for crystallographic phase studies, UV-Vis spectra for band gap analysis, and FT-IR for functional group analysis.

Keywords: Li_4SiO_4, Li-ion, XRD, UV-Vis, FT-IR

Functional behavior of Nb doped LLZO garnet solid electrolyte

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ABSTRACT

Technology advancement is largely dependent on the solid electrolyte material used in battery technology. Garnet-type $A_3B_2(SiO_4)_3$ (LLZO) has been proposed as a solid electrolyte for extremely safe Li-ion batteries, with the goal of enhancing battery functions such as flexibility, cycle durability (battery life), recharge time, power density, safety, and other characteristics as well as research techniques and applications. In this study, the synthesised LLZO using a traditional solid-state reaction method and added dopants of Niobium (Nb) in various ratios. The presence of LLZO cubic garnet was demonstrated by the X-ray diffraction (XRD) patterns. Fourier transform infrared spectroscopy (FTIR) and UV-vis spectroscopy were also utilised to examine the electrolyte's optical band gap. Techniques for LLZO synthesis and characterization are addressed in this work.

One-step synthesis of visible-light responsive Tungsten doped TiO_2 nanospheres for Tetracycline mineralization under visible light irradiation

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ABSTRACT

A set of Tungsten doped TiO_2 (W@TiO_2) nanoparticles were successfully synthesised by a non-surfactant assisted single-pot sol-gel method and utilized for the photocatalytic removal of tetracycline in aqueous medium. The prepared materials were investigated for their physiochemical properties by various analytical methods. The sol gel synthesized TiO_2 showed the presence of both rutile and anatase phases as evident from the XRD analysis. After tungsten doping, the formation of rutile phase in TiO_2 was completely restricted. An orderly arranged nanospherical morphology of TiO_2 particles with well resolved grain boundaries was clearly shown in the Scanning and Transmission Electron Microscopic images. The optical properties studied by UV and PL methods indicated the visible light absorption of materials with reduced bang gap energy and lower recombination rate of the photogenerated charge carriers. With increased amount of W in the samples, the recombination rate of electron hole pairs in the composites was decreased. Under visible light irradiation, 98 % TC was removed with an initial concentration of 25 mg/L for a catalyst dose of 100 mg for 8%W doped TiO_2 sample. The enhanced activity of the W@TiO_2 sample could be due to the increased life time of the charge carriers developed in TiO_2 after the addition of Tungsten. Photogenerated holes and hydroxyl radicals played superior role in the TC mineralization as evident from the scavenger studies. Moreover, the catalyst was successfully reused five times for the TC degradation without a severe loss in the performance.

Keywords: Aquatic pollution; Electron-hole pair separation; Photocatalysis; TC mineralization; Hydroxyl radicals; Sol gel TiO2

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Anomalous behaviour of magnetic coercivity in three dimensional Graphene networks

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ABSTRACT

In this work, the porous graphene has been successfully prepared using hydrothermal method with various concentration of Graphene Oxide (GO) water suspension. The porous nature of graphene was characterized by FESEM, Powder XRD, Raman and FTIR analysis. The defect on the surface of the sample was analysed by XPS and EPR studies. The magnetic properties of porous graphene were investigated experimentally using vibrating sample magnetometer. A strong diamagnetism accompanied by weak ferromagnetism was observed in GO at room temperature. However, when the functional groups were removed from the GO using hydrothermal reduction, ferromagnetism was observed at room temperature. The porous graphene having Coercivity of 710 Oe and saturation magnetization of 0.0168 emu/g were achieved. Higher coercivity in porous graphene network may be attributed to the reduction of GO with increased defect density and remaining sp3-type epoxide groups attached on the basal plane of porous graphene.

Efficient removal of Fuchsine Basic from aqueous solution by Activated Carbon of *Varagu Millet Husk* – Equilibrium and Kinetic Studies

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ABSTRACT

Black Gram belongs to the family *Leguminoseae* bearing the botanical name as *Vigna mungo L*. It is one of the important pulse crops in India. A novel adsorbent of activated carbon with efficient adsorptive removal was prepared by using Varagu Millet husk impregnated with phosphoric acid. ACVMH) tested for their surface functional groups proved the presence of O-H stretching vibrations and C-O, C= O stretching. X-ray diffraction study revealed that the adsorbent is graphitic and crystalline in nature. The surface area of the ACVMH determined by Brunauer Emmet and Teller method is 397.33 m^2/g. and the mesopore volume is 97.91 %. Investigation on various parameters like the effects of contact time, adsorbent dose and initial dye concentration at different temperatures for Fuchsine basic(FB) was done. Among the isotherms the Langmuir model gave the best fit for the uptake of FB dye with the adsorption capacity 3.832 $x10^{-4}$. In adsorption kinetics it was observed that the adsorption of FB dye followed the pseudo-second-order model.

Keywords: Varagu millet, Fuchsine Basic, Activated carbon, Kinetics, Isotherms

Enhancing Bifunctional $CuCo_2S_4$ nanoparticles for high performance all-solid-state asymmetric supercapacitors and efficient electrocatalyst for oxygen evolution reaction

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ABSTRACT

Bi-functional $CuCo_2S_4$ nanoparticles is an emerging electrode material for energy conversion and storage technology due to their crystal structure, and tunnel bandgap and unique morphologies. Ternary $CuCo_2S_4$ nanoparticles has been reported in energy storage device such as lithium-ion batteries and supercapacitors but it is never been reported as catalyst materials for electrocatalysis applications. Unrevealing the microstructure and morphologies of the materials will be an effective method to enhance the electrochemical performances. Herein, the bi-functional $CuCo_2S_4$ nanoparticle is synthesized by a one-pot protocol for elucidating their utilization as the electrode for supercapacitors and oxygen evolution reaction (OER). The electrochemical investigations depicted that the $CuCo_2S_4$ nanoparticles exhibited excellent supercapacitor performance as well as basic OER electrocatalytic activity than that of pure CuS and CoS nanoparticles. In addition, an all-solid-state supercapacitor was assembled, which delivered a high-power density of 4590 W kg^{-1} at an energy density of 25.77 Wh kg^{-1} with a retention of 95% after 5000 cycles. Furthermore, $CuCo_2S_4$ nanoparticles demonstrated excellent electrocatalytic performance with a lower overpotential ($\eta 10$) and Tafel slope values of 330 mV and 76 mV dec^{-1} for oxygen evolution reaction at a current density of 10 mA cm^{-2}, which is superior to that of both of isolated CuS and CoS as well as most reported counterparts. The superior electrochemical performance is due to the synergistic effect of the Cobalt-rich surface, oxygen vacancies, hybridization of Cu-Co and well-defined nanostructure and morphology of the $CuCo_2S_4$ nanoparticles enhancing the active sites that could promote the electrochemical reactions such as supercapacitor and electrocatalysis. This work may inspire the nanorod bundle architecture of bifunctional nanomaterials to achieve performance in cross-field applications.

Keywords: Nanoflakes, electrochemical measurements, hydrothermal method, solid state asymmetric supercapacitors

An investigation into the impact of adding zinc (Zn^{2+}) in manganese ferrite nanocomposite

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ABSTRACT

The Magnetic nanoferrite particles MnZn ferrites are a class of soft magnetic materials that have very good magnetic and optical properties. The manganese zinc ferrite nanocomposite ($Mn_{1-x}Zn_xFe_2O_4$) where, x = 0.25, 0.5, and 0.75 were synthesized by using facile solvothermal technique. The influence of the doping zinc (Zn^{2+}) metal ion in the manganese ferrite nanocomposite was investigated. To study the various structural parameters, the X-ray diffraction and high-resolution scanning electron microscopy were used. The elemental analysis was carried out using energy-dispersive spectrum (EDX). Measurements of the magnetic characteristics, such as magnetization and coercivity, were made using a vibrating sample magnetometer. Nanoparticles were discovered to have lower observed magnetization values than their bulk counterparts. It is possible to have surface effects at the nanoregime due to the variation in lattice constant, decreased magnetization values, variation in magnetization with zinc substitution, and the presence of a net magnetic moment for the zinc ferrite in the $Mn_{1-x}Zn_xFe_2O_4$.

Keywords: MnZn Ferrite, XRD, HRSEM, VSM, Manganese Zinc Ferrite

Hydrothermal Synthesis of Bimetal oxide-based Nanomaterials for Enhanced Supercapacitor Applications

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ABSTRACT

The escalating energy crisis has speed up the development of new energy sources and energy storage technologies. Electrochemical supercapacitors outperform other electrical energy storage devices due to their high power density, fast charge-discharge capability, good cyclic stability, and long life-span. Carbon nanotubes/nanofibers, activated carbon, templated carbon, and reduced graphene oxide have all been extensively studied as electrode materials for double layer-based supercapacitors. However, due to the limitation in effective double-layer area, the specific capacitance of carbon-based materials is generally low in the range of 100-350 Fg^{-1}, limiting their commercial application as supercapacitor electrode materials. Transition metal oxides and conducting polymers promote faradic pseudocapacitance through fast and reversible redox reactions. The hydrothermal method was used to prepare $CuCo_2O_4$ nanomaterials in this study. FT-IR, XRD, SEM, EDAX, Elemental mapping, and Raman analysis were used to investigate the crystallinity, morphology, chemical composition, and other spectroscopic properties of the as-synthesised nanomaterials. The electrochemical properties were also investigated using cyclic voltammetry. Cyclic voltammetry, galvanostatic charge-discharge electrochemical impedance spectroscopy, and cyclic stability studies were used to investigate the improved super capacitor performance of $CuCo_2O_4$. The $CuCo_2O_4$ electrode has a maximum capacitance retention of 95% after 2000 cycles and a maximum capacity of 765 $mAhg^{-1}$ at a specific current of 2 A/g. It also has a high energy density of 25 W h/kg and a high power density of 450 W/kg.

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Phytosynthesis of functionalized gold nanoparticles using blossom extract of Azadirachta Indica and in vitro evaluation of anti-diabetic and antioxidant properties

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ABSTRACT

The current study describes the in situ biosynthesis of gold nanoparticles (AuNPs) with enhanced in vitro anti-diabetic and antioxidant properties using Azadirachta Indica blossom extract. The formation of AuNPs was confirmed by the characteristic optical response through the surface plasmon resonance (SPR) band (454 nm). Using the SPR band, the effect of reaction parameters such as temperature, pH and precursor concentration on the size and surface morphology of AuNPs was optimized. X-ray photoelectron spectra (XPS) results proved the metallic form of phytosynthesised AuNPs with a distinctive binding energy difference of 4f shells $\Delta E = 3.8$ eV. The influence of phytochemicals on the formation of AuNPs was examined through Fourier-transform infrared spectroscopy (FTIR). The structural features were analyzed using transmission electron microscopy (TEM) and X-ray diffraction (XRD) studies. AuNPs showed remarkable antioxidant property compared to the neem blossom extract. The results showed the biosynthesized AuNPs using neem blossom extract demonstrated highly enhanced biological properties for the drug delivery system. **α**-amylase and **α**-glycosidase assays were used to establish the biocompatibility and versatility of AuNPs. The important property of AuNPs for its enhanced plasmon response could be the centre of attraction for its versatility in cutting-edge topics.

Keywords: Gold nanoparticles, diabetic mellitus, XPS, anti-diabetic, antioxidant, phytosynthesis, and neem blossom extract, HRTEM.

Green versus chemical synthesis, physical investigation and biological activities of ZnO NPs using *Curcuma longa* flower extract

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ABSTRACT

Lately, biomedical nanomaterials have received more concerns because of their prominent biological characteristics and biomedical applications. Zinc oxide, a well-known inorganic metal oxide in nanoparticle form, has outstanding antibacterial properties. In this work, the authors focus on determining the anti-bacterial activity of chemically and green synthesized ZnO NPs, respectively. A simple soft chemical route and a green synthesis approach were used to produce chemically synthesized and green synthesized nanoparticles. These samples are investigated and compared in terms of their structural, morphological, optical, and antibacterial properties. The synthesized nanoparticles have a hexagonal wurtzite structure of ZnO, with a crystallite size of 50 nm for C-ZnO and 15 nm for G-ZnO, according to XRD investigations. The presence of bioactive functional groups results in the transformation of bulk zinc acetate to ZnO NPs was also confirmed by FTIR. UV–Vis–DRS spectroscopy was used to investigate optical properties such as reflectance and band gap. The grain size of the synthesized G-ZnO NPs has been decreased, as seen by FESEM and TEM images. The antibacterial efficiency of plant extracts against two different bacterial strains, *S. aureus* and *E. coli*, has been studied and reported.

Stilbene-containing carbazole-based fullerene derivatives as alternative electron acceptor for efficient organic solar cells

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ABSTRACT

We developed novel fluorine and nitro-containing stilbene-linked carbazole-based fullerene (C_{60}) derivatives for bulk heterojunction organic solar cells (BHJ-OSCs). The synthesized fullerene derivatives (**FCzC$_{61}$BM** and **NCzC$_{61}$BM**) have hexyl chains that possess good solubility in toluene and chlorobenzene organic solvents. The extended conjugation of **FCzC$_{61}$BM** and **NCzC$_{61}$BM** molecules showed broad absorption with strong absorption intensity. The **FCzC$_{61}$BM** and **NCzC$_{61}$BM** both have a low-lying lowest unoccupied molecular orbital (LUMO) level of -3.70 eV and -3.75 eV, respectively, due to extended conjugation with electron donor. These LUMO energy level was quite close to the donor (P3HT) LUMO energy level, which is essential for electron transport properties. The BHJ-OSC device were fabricated using **FCzC$_{61}$BM** and **NCzC$_{61}$BM** as the acceptors with commercially available P3HT donor materials using following configurations ITO/PEDOT:PSS/P3HT:**acceptor**/LiF/Al. The **FCzC$_{61}$BM-**based device showed a maximum *PCE* of 0.86% with J_{sc} of 8.36 mA/cm^2, V_{oc} of 0.34 V and *FF* of 0.30. These findings clearly demonstrated that the inclusion of stilbene and carbazole in C_{60} acceptor derivatives exhibited superior optical and electrochemical properties, as well as photovoltaic performance. These findings will help to rationally design the new C_{60} acceptor for OSC applications in the near future.

Keywords Organic solar cells. Carbazole. Electron acceptor. Fullerene derivatives.

Synthesis, characterization, and biological evaluation of copper-nickel mixed metal oxide nanoparticles via a green route using *Cypostemma setosum* L. leaf extract

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ABSTRACT

In recent years, the development of green synthesis methods for the production of metallic nanoparticles has gained considerable attention due to their eco-friendliness and potential applications in various fields. In this study, we report the synthesis of copper-nickel mixed metal oxide nanoparticles using Cypostemma Setosum L. leaf extract as a reducing agent. The synthesized nanoparticles were characterized using various techniques such as UV-Vis spectroscopy, X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, transmission electron microscopy (TEM), and energy-dispersive X-ray spectroscopy (EDX). UV-Vis spectroscopy analysis confirmed the formation of nanoparticles with a surface plasmon resonance (SPR) peak at 488 nm. XRD analysis revealed the crystalline nature of the nanoparticles with a mixed metal oxide structure. The FTIR spectra showed the presence of functional groups involved in the reduction and capping of nanoparticles. TEM analysis showed that the nanoparticles were spherical in shape with an average size of 20-30 nm. EDX analysis confirmed the presence of copper and nickel in the synthesized nanoparticles. The synthesized nanoparticles were further evaluated for their biological activities such as antibacterial, antioxidant, and cytotoxicity. The antibacterial activity was assessed against two gram-negative bacteria, Escherichia coli and Pseudomonas aeruginosa, and two gram-positive bacteria, Staphylococcus aureus and Bacillus subtilis, using the well diffusion method. The results showed that the nanoparticles had significant antibacterial activity against all tested bacteria. The antioxidant activity of the nanoparticles was evaluated using the DPPH assay, and the results showed that the nanoparticles had potent antioxidant activity compared to the standard antioxidant, ascorbic acid. Furthermore, the cytotoxicity of the nanoparticles was evaluated against human breast cancer cells (MCF-7) using the MTT assay. The results showed that the nanoparticles had significant cytotoxicity against MCF-7 cells with an IC50 value of 15 µg/mL. In conclusion, the green synthesis of copper-nickel mixed metal oxide nanoparticles using Cypostemma Setosum L. leaf extract is an eco-friendly, cost-effective, and efficient method for the synthesis of nanoparticles with potential applications in biomedical and industrial fields. The synthesized nanoparticles showed significant antibacterial, antioxidant, and cytotoxicity activities, which make them promising candidates for further studies.

CHITOSAN BASED SEMI- INTERPENETRATING POLYMER NETWORKS AS ADSORBENTS

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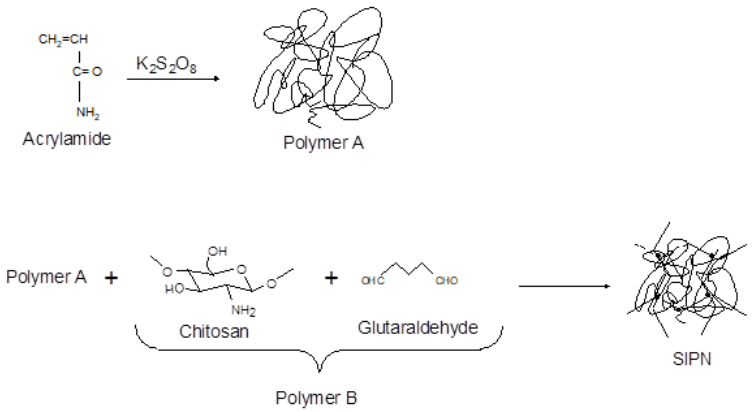
ABSTRACT

The accumulation of heavy metal ions is of great concern to humanity [1]. It is desirable to develop new adsorbents which could be used for removing metal ions from waste water because adsorption is fast, low cost and is efficient [2]. A semi-interpenetrating polymer network (SIPN) consisting of chitosan and polyacrylamide was successfully synthesised and characterised.



Scheme 1. Synthesis of chitosan-polyacrylamide SIPN

The metal ion uptake property of this SIPN was explored in detail towards Cr(VI), Fe(II), Co(II), Ni(II), Cu(II) and Zn(II) ions . Parameters like pH of the solution, concentration of the metal ion solution, and temperature were found to control adsorption processes. The binding of metal ions was investigated using various adsorption isotherms and Freundlich isotherm could satisfactorily explain the experimental data. The possibility of SIPN to be used as an effective adsorbent was evidenced from the selectivity towards Cu(II) from simulated waste water. The study showed that SIPN could be used as an efficient adsorbent material for the removal of metal ions from aqueous solution.

Keywords: Adsorption, Chitosan, semi-interpenetrating network, Polyacrylamide, Metal uptake, Biosorption, Selectivity

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Synthesis, Characterization, and Biological Application of Copper Nanoparticles Encapsulated with Toluene-Soluble Constituents of Solanum Virginianum Plant Extract

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ABSTRACT

Copper nanoparticles (CuNPs) have gained significant attention due to their unique physicochemical properties and various potential applications in different fields. In recent years, the use of plant extracts for the synthesis of CuNPs has emerged as a sustainable and eco-friendly approach. Solanum Virginianum is a medicinal plant known for its various pharmacological properties. In this study, we synthesized and characterized CuNPs encapsulated with toluene-soluble constituents of Solanum Virginianum plant extract and evaluated their biological activity. The synthesis of CuNPs was carried out by reducing copper sulfate with sodium borohydride in the presence of the toluene-soluble constituents of the plant extract. The synthesized CuNPs were characterized using various techniques such as UV-Vis spectroscopy, transmission electron microscopy, and Fourier-transform infrared spectroscopy. The results showed that the CuNPs had a spherical shape with an average size of 10-20 nm and were stable over an extended period. The toluene-soluble constituents of the plant extract acted as reducing and capping agents during the synthesis process, leading to the formation of stable and well-dispersed CuNPs. The Fourier-transform infrared spectroscopy analysis showed the presence of various functional groups such as carboxylic acid, amine, and hydroxyl groups, which played a significant role in stabilizing the CuNPs. The synthesized CuNPs were evaluated for their biological activity using different assays. The CuNPs showed excellent antioxidant activity in the 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay, with an IC_{50} value of 27.3 µg/mL. The CuNPs also exhibited excellent antibacterial activity against Gram-negative bacteria Escherichia coli and Gram-positive bacteria Staphylococcus aureus, with a minimum inhibitory concentration (MIC) of 0.625 mg/mL and 1.25 mg/mL, respectively. The encapsulation of CuNPs with toluene-soluble constituents of Solanum Virginianum plant extract has not been reported before, and this study highlights the use of natural compounds for the synthesis of stable and biologically active CuNPs. The results of this study suggest that the synthesized CuNPs have the potential for various applications in the field of medicine, biotechnology, and environmental remediation. Further studies are needed to evaluate the in-vivo toxicity and biocompatibility of the synthesized CuNPs for their safe use in different applications.

SUITABILITY EVALUATION OF MAGNESIUM ALLOY FOR BIOMEDICAL IMPLANTS

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ABSTRACT

Magnesium (Mg) and Mg alloys are potential candidates for biomedical applications because of their high specific strength, low density, elastic modulus, degradability, good biocompatibility and biomechanical compatibility. The magnesium based alloys possess a natural ability to become biocompatible with the muscular tissues. It undergoes osseointegration and biodegradation due to corrosion when exposed to aqueous substances such as human body fluids and blood. It proves to be a promising candidate for cardiovascular and orthopaedic medical applications. It is a better choice over other metals such as titanium, stainless steel, cobalt-chrome, etc., for the application of permanent implants. It also removes the process of secondary surgery for removal of implant after the patient's recovery. These implants are absorbed by the body after completing their temporary functions, like mechanical support, scaffolding, and binds itself to the living tissues. A novel magnesium alloy was developed with features like good resistance towards fatigue, stress, deformability, and corrosion. It is essential to understand the metallurgical as well as mechanical characteristics to improve their functionality and biocompatibility. The antibacterial activity was studied in order to understand the suitability for patients of all categories.

Optical Properties of Ag Doped Tio2/Sno2 Composite for Solar Cell Application

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ABSTRACT

With the aim of designing high efficient Dye Synthesized Solar Cells (DSSC), Ag doped TiO_2-SnO_2 nanocomposites is prepared by hydrothermal method. The synthesized nanostructures are characterized by basic characterization techniques such as XRD, EDS-SEM, FTIR, Raman spectroscopy and UV-visible spectroscopy. The XRD pattern affirmed that the obtained nanostructures have a tetragonal structure. No regular shape morphology could be seen in SEM analysis. Modification of TiO_2 and SnO_2 by Ag doping led to a slight decrease in the specific surface area. FTIR and Raman analysis confirms the presence of disorder in SnO_2 nanostructures by the doping with Ag in SnO_2 and TiO_2 and also (TiO_2+SnO_2) nanostructures. It was found that absorption properties of the obtained nanocomposites are better towards than pure TiO_2 and SnO_2 nanoparticles. Ag doped (TiO_2 + SnO_2) composite may offer a new potential route for designing cost-effective, highly stable and efficient DSSCs.

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Aqueous room temperature synthesis of nano calcium metal organic frameworks for nitrobenzene detection

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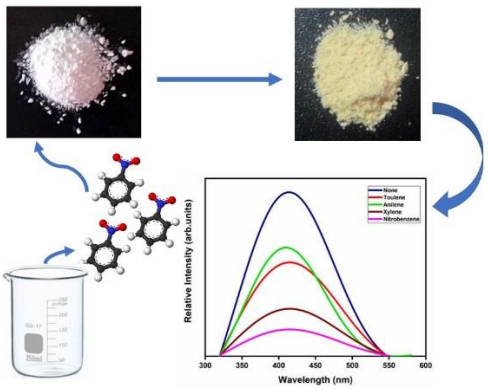
ABSTRACT

A novel Calcium based nano metal organic framework, $[Ca_4(phdc)_3(H_2O)_6]$ has been synthesized by the self-assembly of 1,2-phenylene diacetic acid (phdc) and $CaCO_3$ at room temperature with ultrasound assistance in aqueous media. The synthesized nano material was characterized by FT-IR spectroscopy, Powder X-Ray Diffraction (PXRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), thermogravimetric analysis (TGA), PL spectroscopy and elemental analysis. The synthesized nano MOF is showing high chemical stability in most of the organic reagents and thermally stable up to 370 °C. The photoluminescence study indicates fluorescent properties making it a potential candidate for application in photoactive materials and it will be a good candidate for detection of nitrobenzene explosives in vapor phase based on fluorescence quenching.

Keywords: Metal organic frameworks, Ultrasonic synthesis, Sensing, Nitrobenzene detection



Graphical ABSTRACT

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"EDM Machining Performance of Al-Cu-ZrB2 Nano-Composite Electrodes and Optimized Wear Rate Analysis of SS205"

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ABSTRACT

EDM is a type of machining that relies on the thermoelectric energy of the material and the cutting electrode. EDM is one type of unconventional machining technique. The impact of the input parameters and navel Nano electrodes used in SS205 electric discharge machining are evaluated in this study. During this phase, successive, independent discharges between the electrode and the workpiece help to remove the product electro thermally and using EDM oil as a dielectric fluid and input parameters like current, pulse on, and pulse off.. The Taguchi L9 method, the electrode content, and the SS205 electrode workpiece manufacture are employed for experimentation, with ANOVA analysis being applied for optimization. Choosing the right electrode could lower machining costs. Therefore, die-sinker EDM using an Al-Cu-ZrB2 composite electrode can lower wear and manufacturing costs. The following input parameters need to be used in order to attain a low wear rate: The wear rate is 0.0006 mm3/min, Ton is 50µs, Toff is 80µs, and SV is 12 amps.

Keywords: EDM, Electrodes, Materials, Performance, Wear rate, ANOVA.

"Parameter optimization and Removal Rate Cu-Ni-B4C metal matrix composite as an EDM electrode With D2-Die Steel"

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ABSTRACT

The performance of the electrode materials and process parameters is one of the key factors that affects both the cost of operating the electro discharge machining (EDM) operation and the quality of the machined component. Since copper and graphite electrodes have a limited resistance to electrode wear, sintered composite electrodes had to be created for EDM application. A unique copper-based metal matrix composite (Cu-Ni-B4C) with the best possible balance of wear resistance was the aim of this investigation. Here, Metal Matrix Composite was fabricated using powder metallurgy, and the EDM tests were conducted on test specimens made of D2 tool steel. In this experiment, several input parameters were analyzed to see how they affected the metal removal rate. Following are the EDM process parameters for achieving the Maximum Metal Removal Rate: polarity = positive; SV = 3 V; DC = 8 amps; T ON = 70 s; and T OFF = 80 s. These parameters were also validated through confirmatory experiments.

Key words: EDM, Electrodes, Materials, Performance, Parameters, MRR.

Effect of reinforcement of mixed metal oxide nanoparticles in polyurethane resin for barrier and dynamic mechanical properties of steel structures

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ABSTRACT

Electrochemical techniques were used to study the anticorrosion and mechanical capabilities of the generated polyurethane (PU)/Fe_2O_3-Al_2O_3 nanocomposite coated steel. In natural saltwater, EIS experiments indicated outstanding protective behaviour for the PU/Fe_2O_3-Al_2O_3 coated steel. The coating resistance of the PU/Fe_2O_3-Al_2O_3 nanocomposite was determined to be 18999.17 kΩ.cm^2. The coating resistance of the PU/Fe_2O_3-Al_2O_3 nanocomposite coating was found to be roughly 75% higher than that of the PU coating. The perceived current by SECM analysis across the PU/Fe_2O_3-Al_2O_3 coating was 1.7 nA. SEM/EDX and XRD analyses of the coated steel surface revealed that the Fe_2O_3-Al_2O_3 was accumulated at the corrosion products, preventing the corrosion. Salt spray analysis was used to learn more about the protective properties of coatings. Dynamic mechanical analysis revealed that when the nanoparticle concentration was 3 wt%, the PU/Fe_2O_3-Al_2O_3 nanocomposite coating had improved dynamic mechanical parameters. The aggregation of Fe_2O_3-Al_2O_3 in the PU coating, however, resulted in deterioration in mechanical characteristics beyond 3 wt%. The PU/Fe_2O_3-Al_2O_3 nanocomposite had a good hydrophobic behaviour (WCA: 141^o). The newly synthesised PU/Fe_2O_3-Al_2O_3 composite offered great barrier and mechanical properties, preventing material degradation and increase the lifespan of the coated steel, according to the electrochemical and mechanical investigations.

Keywords: Dynamic mechanical properties; Fe_2O_3-Al_2O_3; Nanocomposite; Coatings and Corrosion; Adhesion; electrochemical techniques; Polyurethane

Novel multilayer structural epoxy nanocomposite coating for enhanced adhesion and protection properties of steel

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ABSTRACT

This work is aimed to synthesize novel structural epoxy nanocomposites containing graphene oxide (GO) and 3-(trimethoxysilyl)propyl methacrylate (TSM) modified W_2N. The protective performance of epoxy coating on mild steel in the presence of different concentrations of GO/TSM-W_2C was evaluated in seawater by electrochemical impedance spectroscopy (EIS) and scanning electrochemical microscopy (SECM). The EIS measurements showed an enhanced coating resistance of EP-GO/TSM-W_2N nanocomposite (22565 kΩ.cm^2) after 20 d immersion seawater compared to pure epoxy (1.01 kΩ.cm^2) coatings. It was also found that the coating resistance of EP-GO/TSM-W_2N was over 79 % higher than that of pure matrix. SECM measurements detected the least dissipation of ferrous ions at the crack of the EP-GO/TSM-W_2N nanocomposite coated steel specimen (1.3 I/nA) due to the improved resistance for anodic dissipation of the coated substrate. FE-SEM/EDX examined that W_2N was reinforced in the degradation products which formed an excellent passive layer at the coating/steel interface. The results showed that the newly developed EP-GO/TSM-W_2N nanocomposite coating possessed superior corrosion protection and enhanced hydrophobic behaviors (WCA: 161º). The investigated coatings showed profound mechanical properties. The inclusion of graphene oxide wrapped W_2N in the epoxy matrix displayed superior mechanical properties in term of adhesion strength and hardness.

Keywords: Epoxy matrix; Graphene oxide; Coating and corrosion; W_2N; Nanocomposite; Adhesion

Multilayered nanocomposite coatings for enhanced anticorrosive, flame retardant and mechanical properties in automobile and aerospace industries

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ABSTRACT

The anticorrosion, flame retardant and mechanical properties of polyurethane (PU) coatings have been improved by the integration of Tantalum disulphide (TaS_2), 2,5-Bis(4-aminophenyl)-1,3,4-thiadiazole (BAT), reduced graphene oxide (rGO). The structural, morphological, and dielectric behaviours of the films were characterized for the different formulations of coatings such as pure PU, PU-TaS_2, PU-BAO/TaS_2, PU-rGO/TaS_2 and PU-rGO/BAT-TaS_2 by means of SEM/EDX, TEM, TGA, XPS, and XRD techniques. As a result, with the addition of only 0.3% rGO/BAT-TaS_2, the dielectric constant of PU was increased by 86-fold at 10 Hz. Additionally, the PU-rGO/BAT-TaS_2 had significantly lower PHRR and THR values than pure PU, a difference of 67% and 61%, respectively, demonstrating its greater flame retardancy. The electrochemical techniques and mechanical testing confirmed that rGO/BAT-TaS_2 (0.3%) composite exhibit enhanced anticorrosive, hydrophobic, flame retardant, and mechanical performance of the PU coating. The super hydrophobic behaviour is confirmed by its WCA of 165˚. Furthermore, the resistance of the PU-rGO/BAT-TaS_2 was found to be much higher (23985.6 $k\Omega.cm^2$) than that of the pure PU (145.4 $k\Omega.cm^2$) and the microhardness and tensile strength were increased sharply. Therefore, the PU-rGO/BAT-TaS_2 nanocomposite could act as a potential coating material for industrial applications.

Keywords: Reduced graphene oxide; *Nanocomposite; Corrosion;* Surface analysis; Flame retardant

Investigation of Turning Parameter on Al-SiC-CuSn-Zn Metal Matrix Composite

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ABSTRACT

When compared to metals, MMC (metal matrix composites) have better mechanical qualities for a variety of applications. As a result, MMC started to be used as a very good metal substitute in a wide range of mechanical applications. A summary of the turning of reinforced particles comprised of 83% strengthened aluminium, 10% bronze, 5% silicon carbide, and 2.5% zinc is given in the publication. Here Cutting speed, feed rate, and depth of cut are the input parameters for this CNC turning process. The research also emphasises how reinforced MMC has recently evolved from modern hybrid composites. Tool wear rate, and material removal rate are only a few response variables that are shown in this article to be affected by various machining factors. Based on the Taguchi L9 Method, this paper discusses the temperature and hardness of the working materials. From the analysis we obtained optimum parameters for achieving best performance from feed rate 0.100 mm/Rev, speed 800,1000 and 1200 rpm, Depth of Cut 0.15,0.25 and 0.35mm we are obtained MRR is 0.0328 gm/min. for optimization technique here we used ANOVA.

Keywords: MMC, Cutting speed, Feed, Depth of cut, Machinability, MRR, ANOVA etc.

SYNTHESIS AND CHARACTERIZATION OF CREATININIUM BENZENE SULPHONATE SINGLE CRYSTAL

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ABSTRACT

Creatininium Benzene Sulphonate crystal is grown by solution growth method using slow evaporation technique. The single crystal powder XRD is taken Creatininium Benzene Sulphonate to obtain the lattice parameters and also to identify the planes present in the crystals. The functional groups of both Creatininium Benzene Sulphonate are analysed through FTIR spectrum. The UV-Vis-NIR study reveals the optical property of the grown CRBS. The hardness behaviour of the crystals is confirmed by Vickers microhardness test.

Keywords: Crystal growth, Creatininium benzene sulphonate, XRD, FTIR, Micro hardness, UV, Non-linear optical .

STRUCTURAL CHARACTERIZATION STUDIES ON THIOUREA DOPED DIGLYCINE PICRATE: A NON LINEAR OPTICAL

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ABSTRACT

The crystal of DiGlycine Picrate (glycine glycinum picrate) has been obtained from an aqueous solution containing stoichiometric quantities of the components. Thiourea was doped with DGP and the crystal structure was determined with high accuracy, IR spectra were taken and compared with the results of DGP. DiGlycine Picrate (DGP) and Thiourea doped DGP crystals were grown by solution growth method using slow evaporation technique. The lattice parameters are obtained through single crystal XRD study. The powder XRD spectrum helps to prove the crystalline nature of the crystal and also to identify planes present in the crystals. The UV- Vis-NIR study reveals the optical property of the grown crystals. The hardness behaviour of the crystals is analyzed by using Vickers micro hardness test.

Keywords: Crystal growth, Glycine picrate, Thiourea, XRD, FTIR, Hardness, Non linear optical.

A STUDY ON CATION EXCHANGE CAPACITY OF PLANT COMPOSITE

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ABSTRACT

Heavy metals play crucial role in the water pollution as they are non-biodegradable. Their multitudinous agricultural domestic, industrial and medical applications have lead to extensive distribution in the environment. These heavy metals pose a hefty threat to the environment and so these metals need to be removed from the waste water effluent. Removal of heavy metals is a challenging process and it requires continuous monitoring and attention. Ion -Exchange method is one of many techniques used in the treatment of water. A few composite ion exchangers were prepared by blending sulphonated carbon from *Diospyros Ebenum* blended with Resorcinol-Formaldehyde resin (RFR) in different weight ratio (0 to 50%w/w). These composites were used as ion-exchangers for the removal of some selective heavy metal ions (Hg2+ Pb2+Cu2+, & Zn2+). The composites were insoluble in various organic solvents and are were thermally stable and stable towards various reagents. It was found that the composites up to 30% (w/w) blending retained the essential properties of original RFR. Hence these composites could be used as lowcost ion-exchangers, when sulphonated *Diospyros Ebenum* partly replaces the original *RFR* up to 30% (w/w) blending without affecting the properties of RFR.

Keywords: Resorcinol-Formaldehyde Resin-Sulphonated *Diospyros Ebenum*-composite resins heavy metals-cation exchange capacity

Microwave Assisted Synthesis, Spectral, XRD Characterization and Biological Screening of New Co(II) and Ni(II) Complexes of Isoniazid

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ABSTRACT

The Isoniazid (INH) is an antibiotic naturally identical chemically synthetic antituberculosis drug. The metal-organic framework complexes of Co(II) and Ni(II) with isoniazid and oxalate ions as ligands utilizing microwave irradiations have been synthesized and investigated. These compounds have been characterized by elemental analysis, Molar conductance, UV-Visible, FT-IR spectral techniques and XRD studies. From the XRD data analysis various parameters such as lattice parameter, lattice type, and crystal system and particle size have been predicted. Particle size is found to be in the range of nanometer are having the monoclinic structure with well-defined crystalline nature of the synthesized complexes. The electronic spectrum reveals the both of these complexes have octahedral structure. The in-vitro biological screening effect of the investigated complexes were tested against the bacterial agents; *Escherichia coli, Actinobacter* and *salmonella* and against fungal agents *C.albicance* by the disc diffusion method. The compounds have significant antibacterial and antifungal activities compared to the uncomplexed ligand.

Keywords: Isoniazid, Oxalate, XRD, antibacterial and antifungal activity.

Spectroscopic Studies and Biological Evaluation of Vo(II) And Cr(II) Metal Complexes of a Novel Schiff base Ligands Derived from Cinnamaldehyde and Benzenamine

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ABSTRACT

A series of new complexes of the Schiff base obtained from cinnamaldehyde and Benzenamine. The general formula [M (L_1) (L_2)],(L_1- (E-N-(E) -3phenylallylidene)aniline, L_2- oxalate) has been synthesized and characterized with the structure features have been determined from microanalytical, IR,UV-VIS, EPR, CV. Molar conductance, Magnetic Moment and MASS spectral data. The complexes Vo(II) and Cr(II) are octahedral geometry. The biologically screening effects of the investigated compounds were tested against the Bacterial Species *E. coli* and Fungal activity against *Ketoconazole* and anti-oxidant, DNA binding and cleavage study. The Schiff base and their Metal complexes comparison of the inhibition values. Which are indicate that the complexes exhibit higher antimicrobial data.

Eco-Friendly Synthesis, Spectral, Bio-Potential, DNA Binding and Antituberculosis Activities of Ni(II) And Cu(II) Complexes

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ABSTRACT

Microwave technique is one of the eco-friendly techniques used widespread in green synthesis of metal-organic compounds. First transition metal complexes of Ni(II) and Cu(II) synthesized using this technique with organic neutral bidentate ligand isonicotinic acid (INH) and anionic benzoate ion. The synthesized complexes were characterized by micro analytical techniques viz., elemental analysis, metal estimation, magnetic moment (VSM), molar conductance and cyclic voltammeter. The spectral techniques UV-Visible, IR and Far-IR are also used to characterize by the synthesized complexes. The elemental analysis, metal estimation, magnetic moment and UV-Visible spectral data of the complexes indicating their molecular formulae, composition and probable geometry (octahedral for Ni(II) and tetragonally distorted octahedral for Cu(II) complexes). Redox properties and reversibility and feasibility of equilibrium of the synthesized complexes were confirmed by their cyclic voltammogram. Complex formation and metal chelating atom (M-O and M-N) ability of the complexes confirmed by their IR and Far-IR spectral data. The antibacterial and antifungal activities of the ligand (INH) and its complexes were carried out by Agar well diffusion method using Actinobacter, Salmonella, *E. coli* (bacterial strains) and *C. Albicance* (Fungal strains). The DNA binding and cleavage studies of the complexes compared with those for pure ligand using Calf-thymus DNA. The complexes can interact with DNA at higher concentration. The antituberculosis of the complexes against *M.tuberculosis* were performed and compared with the standard and ligand isonicotinic acid.

Design and Analysis of Piston Using Composite Material

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ABSTRACT

In today's world a car is a part of everyone's life and it plays an important role. Here in this paper we focus on IC engine Piston. We have discussed new and improved developments regarding the increased efficiency of IC engine Piston. Also a different type of composite metal matrix is discussed for the design of IC Engine such as piston aluminum and magnesium materials which are considered to be a matrix for the metal matrix composite as they have excellent mechanical and tribological properties when combined with ceramic and other metical. or non-metallic reinforcement. This paper describes the modeling and analysis of the piston structure with various materials. In this research work the engine piston is modeled with CATIA and to obtain the accuracy of the connection results is done via HYPER MESH and then the analysis is performed using ANSYS. Compared to conventional materials a new discovery has a low weight and high strength Using a distorted engineering method, the CAD model of existing piston was developed and a different type of mold was designed to make pistons. Therefore magnesium-based MMCs can be used for air compressor piston application instead of aluminum alloys.e composite material is made and the coating level is calculated. The results were compared with existing materials and found to be enhanced with bronze hybrid composites. Emission testing was also performed and was found to be improved. Microstructure tests were performed to study the composition of compounds. The mechanical properties of the tensile strength and the strength of the compound have been measured. Composition analysis of the composite material was performed and the level of wear was calculated. The results were compared with existing materials and found to be enhanced with bronze hybrid composites. Emission testing was also performed and was found to be improved.

Keywords – Piston,Bronze, Aluminium,hybrid composite, Thermal analysis, ANSYS, Composite Material, Analysis.

Catalytic Synthesis, Sensor, Solvent Effect and DFT Studies of Imidazole Derivatives

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ABSTRACT

The solvent dependent fluorescence behaviour of heterocyclic molecules is an emerging trend in this era. The designing of simple, well-organized and environmentally benign speculative protocol is a massive challenge to chemists to improve the quality of the environment for present and future generation. A series of imidazole derivatives have been designed and synthesized using nano SiO_2 as an efficient catalyst. Synthesized compounds have been characterized by ^{1}H and ^{13}C-NMR spectral studies. The significant features of this nanocatalyst are high product yield, short reaction times and a vast range of substrates usage. Proton and ^{13}C chemical shift of the synthesized compounds were calculated. The absorption and emission properties of imidazole derivatives have been studied in several solvents. Optimization of 4,5-dimethyl-2-phenyl-1- *m*-tolyl-1H-imidazole has been performed by DFT at B3LYP/6-31G (d, p) using Gaussian-03.

Keywords: Sensor, Absorption, Fluorescence, nano SiO_2, DFT, chemical shift.

Nano Ce-Cuo catalytic synthesis and biological studies of Bis dimedone derivatives

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ABSTRACT

Bisdimedone derivatives, acridines, acridinediones, xanthene derivatives show antimicrobial activities against certain bacterial and fungal strains. Xanthenes are important because of their use in medicine and they possess biological activities. Organic molecules containing xanthene moieties are of biological importance and are useful in drug discovery. The xanthenes derivative, (9S)-9-(2-hydroxy-4,4-dimethyl-6-oxocyclohex-1-en-1-yl)-3,3-dimethyl-2,3,4,9-tetrahydro-1H-xanthen-1-one is a selective and orally active neuropeptide Y-Y5 receptor antagonist. Some xanthene derivatives demonstrate photoactivated insecticidal and pest-control activity, and anticancer properties. Heterogeneous Cerium loaded Cuo nanocatalyst perform as an attractive aspirant for synthesis of innovative molecules that leads to the recovery as well as reuse ability of the catalyst without any sustainable loss of activity.

Keywords: Nano catalyst; Bisdimedone; antimicrobial; anticancer.

Removal of heavy metal by using eggshell membrane as low cost Bio-Sorbent

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ABSTRACT

The objectives of this study were to remove heavy metals from waste water through the bio sorption method Biomass materials are relatively inexpensive and available in large quantities worldwide.¬ Egg shell membrane (ESM) was selected and modified to adsorb heavy metals. ESM is capable of binding¬ various metal ions from aqueous solutions . The egg shell is currently used as a source of calcium in animal feeds and human health supplements. Egg¬ shell is composed mainly of calcium carbonate ; it should behave as sorbents. In this studies, two approaches were made in the recovery process namely batch and column methods. The¬ waste water containing 10ppm iron was used as for the iron removal studies using ESM as the adsorbent. The concentration of iron was determined by UV-Visible spectrophotometer. In the case of batch¬ adsorption with egg shell membrane, dosage of ESM is fixed as 0.5g wherein around 80% iron removal is obtained with 325microns filled ESM. The results are explained in terms of increased surface area and higher dosage.¬ In the column procedure, the crushed ESM powder-packed as mini column (diameter 1.5cm, length 5cm)¬ with 325 microns particles were tired. Flow rate of 0.5ml/min was maintained and the effluent was analyzed. The column sorption experiments were performed at room temperature. The column method seems to be less effective under the experimental conditions than the batch method. Results obtained shown that eggshell can remove several metal ions, with great efficiency. The regeneration studies with ESM suggest 2% HCl to be effective eluent.

Keywords: Adsorption, Biosorbent, Egg shell membrane

Mechanical and Metallurgical Properties of Friction Stir Welding on (AZ31B and AZ91) Mg Alloy Metal Plates

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ABSTRACT

Friction Stir Welding (FSW) is a solid-state welding process that has shown great promise for joining light alloys, such as magnesium and its alloys. This ABSTRACT focuses on FSW of two commonly used magnesium alloys, AZ91 and AZ31B. The process parameters, such as rotational speed, traverse speed, and axial force, have a significant impact on the weld quality and properties of the joint. The microstructure of the weld zone and the heat-affected zone (HAZ) is affected by the welding parameters, and can be optimized to achieve desired mechanical properties. FSW has been shown to produce sound and high-strength jointsinAZ91 and AZ31B alloys, with no macroscopic defects or pores. The mechanical properties of the joints, such as tensile strength, fatigue strength, and hardness, can be improved by optimizing the welding parameters and post-weld heat treatment. This ABSTRACT provides a brief overview of the FSW process for AZ91 and AZ31B alloys, and highlights its potential for producing high-quality joints in these materials. This ABSTRACT summarizes the current state of research on FSW of AZ31B and AZ91, including process parameters, microstructure, mechanical properties, and the influence of post-weld heat treatment. The microstructure of the welds was found to be significantly affected by the tool rotation and welding speed. The welds exhibited good tensile strength and ductility, although the strength of the welds was lower than that of the base metal. Post-weld heat treatment was found to improve the mechanical properties of the welds. Further research is needed to optimize the FSW process parameters for these alloys and to investigate the long-term durability of the welds. In summary, FSW of AZ31B and AZ91 magnesium alloys requires careful consideration of welding parameters to achieve high-quality welds with good mechanical properties. With appropriate parameter selection and process optimization, FSWcan be a reliable joining method for magnesium alloys, offering several advantages over traditional welding techniques.

Keywords: Magnesium alloy, Friction stir welding, Fatigue, FSW process parameters, Microstructure, Ductility, Tensile Strength

Enhanced visible light response photocatalytic activity of Bismuth Ferrite nanoparticles *via* Sol Gel Approach

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ABSTRACT

All life on earth depends on water in some way. The twenty-first century presents significant concerns with regard to contaminants and water quality. Innovative and user-friendly methods for creating materials are urgently needed for the process of purifying water. These innovations are anticipated to provide frameworks with desirable characteristics like speed, efficiency, lack of toxicity, healthiest technique, and cost effectiveness.

According to a recent study, Perovskite nanomaterial is a good option for photocatalytic degradation of waste water pollutants. The use of bismuth ferrite ($BiFeO_3$ or BFO), a perovskite material with a rhombohedral framework R3, in the photodegradation of colors is now attracting a lot of attention. The BFO nanoparticles is an excellent photocatalyst because of its multiferroic characteristics, solid photoabsorption, and precious stone structure. Whenever driven to visible light, a photocatalyst created from in this substance proved to really be particularly effective at degrading colors.

In this work, sol-gel synthesis was used to prepare bismuth ferrite (BFO) nanoparticles. X-ray powder diffraction (XRD), UV-Vis diffuse reflectance spectroscopy, high resolution scanning electron microscope/EDS (HRSEM/EDS), and X-ray Photoelectron Spectroscopy were used to evaluate the materials (XPS).

As a consequence, the X-ray Diffraction Pattern verifies that BFO has a rhombic crystalline structure. The band gap energy of the sample is less than 2.3 eV, according to UV Vis DRS spectra. SEM (HRSEM) was utilized to analyze the morphological characteristics of the produced material. The prepared BFO sample's oxidation status is revealed by XPS. The degradation of Rhodamine Blue (RhB) dye during exposure to visible light was used to measure the photocatalytic performance of the synthesized nanoparticles.

Keywords: Water pollution, Bismuth Ferrite, Sol gel, Photocatalysis, RhB.

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Chromene Carbohydrazide- Schiff Base as a turn-off chemosensor for In^{3+} ion and its application to DrG cell imaging

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ABSTRACT

A new 7-(diethylamino)-2-oxo-2H-chromene-3-carbohydrazide design to synthesize a Schiff-based ligand for the selective detection of cations The Schiff base ligand **L** was synthesized for the selective recognition of In^{3+} ions in DMSO:H_2O (7:3, pH = 7.4). Probe **L** exhibits a selective turn-off fluorescence response at 488 nm with In^{3+} ions. By Job's plot and ESI mass analysis, the probe **L** forms a 1:2 stoichiometry complex with an estimated association constant of 4.75×10^4 M^{-2} with In^{3+} ions. Metal induces CHEQ (chelation-caused fluorescence quenching) to reduce the intensity of the probe **L**'s emission. The limit of detection was found to be 4.3 nM; the time response of the sensor is instantaneous; and its reversible nature was confirmed using EDTA additions. For on-site applications, solid substrates (test-strips) were designed and tested for fast, reliable, user-friendly, and real-time sensing of In^{3+} ions. The binding mechanism of probe **L** with In^{3+} ions was investigated using ^1H NMR titration and DFT/TD-DFT studies. Furthermore, we investigated the real-time applicability of Probe **L** in DrG cell lines for live cell imaging applications.

Keywords: Chemosensor; Carbohydrazide; Aluminum; Indium; Cell Imaging; DFT

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Structural, Morphological and Adsorption Properties of Activated Carbon Synthesized from Banana Peel

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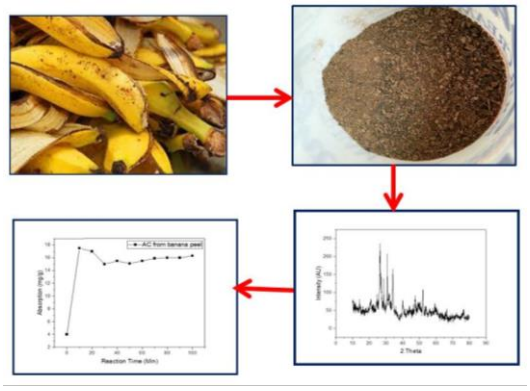
ABSTRACT

The industrial growth in all sectors supports the mankind to create the technically and technologically upgraded society. Supplementary consequences of this rapid growth are environmental pollution. All stages of the ecological system is polluted among them water treatment is the need of an hour and it should be addressed in eco-friendly and economical aspect. Activated carbon prepared from banana peel by chemical activation method. The prepared sample was characterized for structural, morphological and absorption properties. The XRD result shows the polycrystalline nature of the sample and the results suggests that pyrolysis reaction was not complete and amorphous carbon was remained. The surface morphology of activated carbon from banana peel shows improved pore size with dispersed nature. The absorption studies were carried out for Methylene blue which is the major effluent and the cause for water contamination. It was found that the adsorption rate was rapid at first and then attains equilibrium with further reaction time. This results suggests that the activated carbon prepared from bio mass such as banana peel proves to be a better substitute for the waste water treatment.

Keywords: Banana Peel, Activated Carbon, Waste Water Treatment

Graphical Abstract



Influence of Ag/V Co-Doped Hydroxyapatite and its antimicrobial activity

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ABSTRACT

As hydroxyapatite resembles human bone, it has been received the most attention as a biomaterial for use in bone transplants, scaffolds, fillers, cements, coatings, and other procedures to repair and regenerate bone defects. For a tissue engineering scaffold, it is essential to create bone grafts and scaffolds with the appropriate interconnected porosity and adequate strength. Hydroxyapatite is a naturally or synthetically occurring compound. It majorly consists of calcium and phosphate. Doping is one of the effective strategies to improve the strength of the material. The aim of this study was to synthesis pure hydroxyapatite [$Ca_{10}(PO_4)_6(OH)_2$] and Silver (Ag)/Vanadium(V) co-doped hydroxyapatite [$Ca_{10-x}Ag_x(PO_4)_{6-x}(VO_4)_x(OH)_2$] with various concentration such as (x= 0.01, 0.05, 0.1M). Pure Hydroxyapatite and the Silver and Vanadium doped Hydroxyapatite have been synthesized using the chemical precipitation method. Ag^+ and V^{+5} ions replace Ca^{2+} and PO_4^{3-} in hydroxyapatite, respectively. The synthesized samples were characterized using X-ray diffraction (XRD), Fourier transform infrared (FTIR), Field emission scanning electron microscope (FE-SEM), Energy dispersive x-ray analysis (EDX). The antibacterial activity pure and co-doped Hydroxyapatite were investigated.

Amorphous Class of Fe-Al Based Metal-Organic Framework Nanoplates for Rapid Catalytic Decomposition of Azo Dye under Mild Operation Conditions

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ABSTRACT

Efficiently we developed a cost-effective, durable, and stable amorphous class of Fe/Al-based MOF nanoplates. The crucial characterization of powder XRD analysis, HRTEM image, and the SAED pattern evidence the amorphous state of the prepared catalyst Fe/Al-MOF nanoplates. BET results support the presence of mesopores in the amorphous Fe/Al-MOF with a pore diameter of 3.4 nm and a high surface area of 232 m^2/g along with a pore volume of 0.69cc/g. XPS spectrum of Al2p depicts two binding energy values, 74.5 eV accounts for Al-O-Al bonding in alumina, and 74.3eV is attributed to Al-O-Fe linkage. Fe2p portrays the presence of Fe^{2+} (710.1 eV) and Fe^{+3} (713.4 eV) in the Fe/Al-MOF. FE-SEM elemental mapping described the unique distribution of Fe & Al in the framework of aMOF. Catalytic activity was examined toward the destruction of recalcitrant pollutant methylene blue (200ppm) in a batch reactor. The amorphous class of Fe/Al-MOF demonstrated admirable results with 100 % methylene blue degradation and about 78 % Total Organic Carbon (TOC) removal with a negligible quantity of Fe leaching over 45 min. of the treatment at mild reaction conditions. The durability of the catalyst was examined, it displayed about 75 % TOC removal and 100 % methylene blue decomposition over 5 successive recycles with < 1ppm Fe & Al leaching. Based on the above results synthesized amorphous class of Fe/Al-MOF nanoplates proves as a potential candidate for the complete removal of dyes from industrial wastewater.

Keywords: Amorphous Fe/Al-MOF; Heterogeneous Fenton; Advanced Oxidation process; Methylene blue dye degradation; Environmental Remediation

APPLICATION OF ANTIBACTERIAL ACTIVITYAND SYNTHESIS AND CHARACTERIZATION OF ZnO & Mn-ZnO NANOPARTICLES BY FACILE MICROWAVE COMBUSTION METHOD

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ABSTRACT

Using zinc acetate and manganese nitrate and a simple microwave combustion process, manganese doped zinc oxide (Mn-ZnO) nanoparticles were effectively created. The produced samples were evaluated by energy dispersive X-ray (EDX), high resolution scanning electron microscopy (HR-SEM), powder X-ray diffraction (XRD), Fourier transformer-infrared (FT-IR), photoluminescence (PL), and UV-Vis diffuse reflectance spectroscopy (UV-Vis DRS). The powder XRD structural tests show that the produced nanoparticles were well-crystalline and contained a hexagonal wurtzite structure. The uniform spherical morphology of the produced ZnO nanoparticles was confirmed by HR-SEM images. The inclusion of Mn ions in the ZnO lattice was confirmed by EDX analysis. By using UV-Visible DRS spectral analysis to calculate the band gap (Eg) energy, it was discovered that pure ZnO has a lower Eg value than Mn-doped ZnO nanoparticles. The efficient Mn-doping enhances the near band gap emission in the UV and visible regions, according to PL spectra. Mn-doped ZnO nanoparticles shown more effective antibacterial activity than pure ZnO when tested against gramme positive (Bacillus subtilis, Staphylococcus aureus) and gramme negative (Proteus mirabilis, Salmonella typhi) bacteria using optical density measurements.

Keywords: Nanoparticles, Microwave Combustion Method, antibacterial activity, gram positive andgram-negative bacteria, ZnO

Synergistic corrosion inhibition effect and mechanism of halloysite nano clay and polyacrylamide on steel reinforcements in simulated concrete pore solutions

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ABSTRACT

The study examined the combined effect of Polyacrylamide (PA) and Halloysite Nanoclay (NC) in suppressing the corrosion of steel reinforcements in a simulated concrete pore solution. Electrochemical impedance spectroscopy (EIS), linear polarisation resistance, potentiodynamic polarisation, X-ray photoelectron spectroscopy, and molecular dynamics simulations are used here to explore the inhibitive impact on reinforcement corrosion. The NC/PA inhibitor significantly improved anti-corrosive performance in steel reinforcements by the development of a layer that hindered both cathodic and anodic corrosion processes. The obtained electrochemical data demonstrated that adding NC considerably improved PA's inhibition ability. The primary inhibitory mechanism is noticed in the adsorption of corrosion inhibitors on the steel surface, which lowers the corrosion current density of the steel reinforcement.

Keywords: Polyacrylamide; Halloysite nanoclay; Corrosion; Steel; Reinforcements; Concrete; Pore solution; Electrochemical; Adsorption; Inhibitor

Discerning liquid phase oxidation of benzyl alcohol catalyzed by copper aluminate nanostructures

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ABSTRACT

In this work, a simple and economic route for the preparation of CuAl2O4 is proposed. The method was developed with the objective of obtaining a material with greater surface area, when compared to the spinel prepared by conventional combustion method (CCM). The catalytic properties of CuAl2O4 spinel prepared by CCM are compared with the one prepared microwave combustion method (MCM). Nano-sized CuAl2O4 were synthesized by both CCM and MCM using Opuntia dillenii haw as the plant extract, and were characterized by X-ray diffraction analysis (XRD), high resolution scanning electron microscopy (HR-SEM), N2 adsorption/desorption isotherms, and diffuse reflectance spectroscopy (DRS). Oxidation to their corresponding carbonyl compounds, high selectivity, and inexpensive precursors make this catalytic system a useful oxidation method for benzyl alcohol. The XRD results confirmed the formation of a cubic CuAl2O4. The formation of CuAl2O4 nanorices and nanorods structures were confirmed by HR-SEM. Through MCM method, CuAl2O4 (sample B) with a high specific surface area of was obtained. The band gap values of the (2.30 and 2.35 eV) for the obtained oxides are due to the nanometric dimensions of the nanostructures. The effect of the solvent, temperature, and oxidant on the oxidation of benzyl alcohol is reported.

Keywords: Copper aluminate, X-ray diffraction, Nanostructures, Benzyl alcohol, Liquid phase oxidation

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Investigation of the effect of corrosion inhibitors used in reinforced concrete

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ABSTRACT

Corrosion is the natural process of converting a refined metal into a chemically stable ion. Carbonation and chloride or salt attack in corrosion will cause the natural deterioration of metals which affects the service life of the structures. To enhance the service life of the structures, Inhibitors are used. Corrosion inhibitors are chemical substances when added to concrete in the required concentration will inhibit or prolong the time to initiation of corrosion in reinforced concrete structures. According to their action, can be classified into anodic inhibitors, cathodic inhibitors, mixed inhibitors, volatile inhibitors and green inhibitors. In this research, the various types of corrosion inhibitors were evaluated under various conditions by forming a protective film around the embedded steel bars. These are effective in preventing corrosion from reinforced concrete structures. Therefore, the performance and efficiency of the inhibitors strongly depend upon the quality of the concrete and the initial chloride ions concentration in the concrete. Hence it needs more extensive investigation in real concrete structures by considering the various aspects, such as chloride content, type of cement, type of inhibitors, etc.

Keywords: corrosion; corrosion inhibitors; anodic inhibitors; cathodic inhibitors; volatile inhibitors; green inhibitors.

UTILIZATION OF NOVEL HUMAN HAIR AS FIBER REINFORCEMENT IN ORDINARY CEMENT CONCRETE AND INCORPORATION OF CHEMICAL ADMIXTURES AIMED AT IMPROVING THE MECHANICAL PROPERTIES OF CONCRETE

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ABSTRACT

This is a potential area of research to improve the physical and mechanical properties of concrete. Fiber-reinforced concrete (FRC) is a type of concrete that contains fibrous material to strengthen structural stability. Fiber Reinforced Concrete is one of those developments where many forms of fiber are used for this research purpose. This research examines the suitability of human hair. Human hair is considered a waste product in most parts of the world and is a common ingredient found in municipal wastewater streams, causing environmental problems. Generally, human hair fiber is very strong in tension. Experiments were carried out on standard-sized concrete cubes, and prism beams. SPSS Statistical Analysis also derived this comparison value of strength. The addition of Novel Human Hair fiber is 0.5% to 5% in the homogenous mixture of concrete by the weight of cement. M25 grade concrete was used and compared with conventional concrete. 28 days of strength was compared and found the optimal percentage of human hair in concrete. Based on the results of the testing, this research will continue to improve the quality of concrete by including varying percentages of human hair fiber and concrete grades.

Keywords: Novel Human Hair; Fiber Reinforced Concrete, Compressive Strength; Flexural Strength; Air Entraining Agent; SPSS.

A study on the elimination of Pb(II) by Chitosan-g-Poly(Butyl acrylate)/Silica gel nanocomposite

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ABSTRACT

It is indeed an alarming and saddening fact that the wastewater eventually let out by the industries - which contributes very much for the prosperity of the nation - conjoins with the adjacent water sources without proper protection. This study focuses on getting rid of heavy metal Pb(II) present in the water let out by the leather industries with the treatment of Chitosan-g-Poly(Butyl acrylate)/Silica gel nanocomposite (Cs-g-PBA/SG). Although various techniques are there for the treatment of wastewater, adsorption is one of the promising techniques. Batch adsorption study was carried out for the remediation of the wastewater by changing the conditions like adsorbent dose, pH and contact time of adsorption. It is illustrative that the Cs-g-PBA/SG nanocomposite thus obtained can be availed of effectively for eliminating the stalwart metals from wastewater.

Keywords: Tannery Effluent, Physico-chemical variables, Chromium, Wastewater treatment, Polymeric nanocomposite, Chitosan, Silica gel, Kinetics.

PHOTO CATALYTIC STUDIES ON ZINC OXIDE NANOPARTICLES UNDOPED AND DOPED WITH TITANIA AND ZIRCONIA FOR EOSIN YELLOW DEGRADATION

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ABSTRACT

Nanoparticles of Zinc oxide (ZnO) nanoparticles, Titania doped Zinc oxide nanoparticles and Zirconia doped Zinc oxide nanoparticles are synthesised and size characterised using UV-DRS, PXRD, FESEM and EDAX methods. One pot batch type reactor fitted with top view vertical irradiation source was used for dye degradation studies. The irradiation sources are UV and Solar. The catalyst loading was maintained as 1mg/20mL of 1mM Eosin yellow dye aqueous solution. The progress of dye degradation is studied by measuring absorbance versus time intervals at constant wavelength maxima of the dye. Pseudo first order conditions are maintained. Based on the absorbance versus time measurements, the rate coefficient values are determined. The photo catalytic activity of the catalysts in degrading process of the dye is found efficient in solar irradiations. The salient features and results are put forth and discussed.

Keywords: ZnO nanoparticles, Titania doped ZnO nanoparticles, Zirconia doped ZnO nanoaprticles, dye degradation

Electrocatalytic performance of the cobalt oxide nanoparticles decorated graphene oxide for the detection of folic acid

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ABSTRACT

Herein, we designed and synthesized composite material consisting of cobalt oxide anchored on graphene oxide (Co_3O_4@GO) as an electrode modifier, and their application to the detection of folic acid (FA) was investigated. The integration of Co_3O_4 and GO by hydrothermal assisted synthesis route. The morphology and crystalline structure of the Co_3O_4@GO was well analyzed by XRD, XPS, FESEM, HR-TEM, and EDX analysis. The electrochemical test of the Co_3O_4@GO modified electrode shows an interesting electrochemical performance for the selective determination of FA with a broad concentration range of 0.1-4000 µM and a lower detection limit (LOD) of 0.024 µM. The enhancement in the catalytic activity of Co_3O_4@GO can be achieved by the synergistic effect of Co_3O_4 and GO, high electron transportation, and unique spherical structure of Co_3O_4@GO. The newly developed Co_3O_4@GO sensor also displayed excellent sensitivity of 47.23 $\mu A \mu M^{-1} cm^{-2}$. Finally, this Co_3O_4@GO sensor was demonstrated for the detection of FA in the human urine sample with excellent recovery.

Keywords: Folic acid; cobalt oxide; GO; modified electrode; electrochemical detection.

A Biocompatible Electrochemical Sensor Based on PtNi Alloy Nanoparticles Coupled N-GQDs for I*n Situ* Monitoring of Dopamine in Glioma Cells

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ABSTRACT

We report the design and construction of enzyme-free sensors using Platinum-Nickel (PtNi) bimetallic alloy nanoparticle-conjugated nitrogen-doped graphene quantum dots (N-GQDs) for the highly specific *in situ* monitoring of Dopamine (DA) secreted by glioma cells (C6). PtNi@N-GQD nanocomposites were synthesized using a simple ultrasonication method. The resulting hybrid material was an excellent electrocatalyst for the redox activity of DA owing to the combined properties of PtNi alloys and highly conductive N-GQDs. The PtNi@N-GQDs-based sensing platform demonstrated substantial sensing ability, with a detection range of 0.0125–952 µM, a sensitivity of 0.279 µA μM^{-1} cm^{-2}, and a limit of detection of 0.005 µM (S/N = 3). The sensing performance of PtNi@N-GQDs was highly stable, selective, and reproducible. We successfully showed the practical application of the PtNi@N-GQDs sensor by quantifying DA in the blood serum and human urine samples. Finally, we used the PtNi@N-GQDs biocompatible platform to quantify DA released from C6 cells.

Keywords: Neurotransmitter; Dopamine; N-doped graphene quantum dots; Glioma cells; Enzyme-free sensor

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Preparation and Characterization of MnS nanofiller reinforced Polyaniline matrix

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ABSTRACT

The manganese sulphide nanoparticles has been synthesis by hydrothermal process. The MnS-PANI 1, 5, 15 wt. % was synthesised by polymerisation process. The structural parameters of the prepared materials were confirmed by using the Powder X-Ray of Diffraction method. All peaks were exactly matches with JCPDS Card No # 89-4952 confirms the cubic structure of prepared MnS nanoparticle. The high resolution scanning electron microscope (HR-SEM) was used to record the surface morphology. Using the tauc plot the band gap was determined from the UV-Visible (UV-Vis) absorption spectra obtained recorded in the wavelength range of 200-1200 nm. The functional group analyses were carried out by the FTIR spectra. The LCZ characteristics of dielectric loss, dielectric constant, AC conductivity, impedance, and DC conductivity were measured at room temperature, 50 °, 100 °, and 150 °C at a frequency of 1 Hz-1 MHz.

Keywords: Powders: Chemical preparation, Dielectric properties, Metal chalcogenides

Assessment of groundwarter quality during pre-monsoon and monsoon seasons at North Chennai in Tamilnadu, India

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ABSTRACT

This present study deals with the physico-chemical parameters of 50 groundwater samples in North Chennai, Tamil Nadu, India, during pre-monsoon and monsoon periods. The present study combines BIS guideline values, GIS, WQI, Correlation coefficient, Piper diagram, SAR, percentage Na and electrical conductivity to study the groundwater quality in the study area of North Chennai for drinking and irrigation purposes. The study was carried out using Arc GIS to map the water quality to evaluate the spatial deviation of groundwater quality. The physico-chemical study, shows the values of Na, Cl, and EC, exceeding the allowable limits of BIS in both seasons. It is noted that total dissolved solids value in pre-monsoon (30%) and monsoon (37%) pre-monsoon phases exceed the permitted maximum value of 2000 mg/L (BIS). It is observed that EC data in pre-monsoon (96%) and monsoon (90%) seasons are crossing the desirable limit of BIS. Also, the data obtained clearly emphasize the necessary and essential method to rectified the problems. WQI study shows 64% samples of the study area in pre-monsoon and monsoon seasons is unfit for drinking. It shows a good agreement between GIS, WQI, Correlation coefficient and PIPER diagram findings. USSL and Wilcox diagram study clearly agree with each other and disclose that NaCl is the dominant type of the groundwater of the area of investigation and it is clear that the high concentration of sodium chloride is because of the seawater percolation.

Keywords: Groundwater, drinking water quality, water quality index, geographical information system, pre-monsoon and monsoon.

TISSUE ENGINEERING NEEDS NEW BIOMATERIALS: POLY (XYLITOL-CITRATE-SEBACATE) AND ITS NANOCOMPOSITES

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ABSTRACT

Introduction/Background: Poly (xylitol-citrate-sebacate) is recognized as an effective polymer for bone tissue engineering and drug delivery systems owing to its biocompatibility and biodegradability. However, due to a lack of bioactivity and antibacterial activity, its biological applications are hampered.
Methods: In this investigation, Poly (xylitol-citrate-sebacate) (PXCS) was afforded a biosorption increase by the addition of strontium doped mesoporous bioactive glass nanoparticles (Sr-MBGN). In the present study, porous (about 70 vol%) nanocomposite scaffolds made of PXCS and (5 wt%) of Sr-MBG nanoparticles (with a particle size of about 25 nm) containing 5 wt% strontium (Sr) were fabricated by solvent casting technique for bone tissue engineering.
Results: A new xylitol-based Poly (xylitol-citrate-sebacate) and its strontium doped mesoporous bioactive glass nanoparticles were synthesized. Structural characterization was done using high resolution scanning electron microscopy (HRSEM), fourier-transform infrared spectroscopy (FTIR) and tensile test were used to characterize the fabricated samples. In vitro experiments including degradation, bioactivity, and biocompatibility (i.e., cytotoxicity, alkaline phosphate activity, and cell adhesion) tests of the fabricated scaffold were performed. The biomedical behavior of the fabricated PXCS based composite scaffold was interpreted by considering the presence of the porosity, Sr-substituted Sr-MBG nanoparticles.
Conclusions: The fabricated porous PXCS/SrMBGN nanocomposite containing 5 wt% SrMBG nanoparticles could be utilized as a good candidate for bone tissue engineering.

Keywords: Poly (xylitol-citrate-sebacate); strontium doped mesoporous bioactive glass nanoparticles; scaffolds; tissue engineering;

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Impact of Soil-Structure Interaction on the Seismic Response of Regular and Irregular RC structures

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ABSTRACT

The effects of soil-structure interaction (SSI) on the dynamic response of a reinforced concrete wall-frame dual framework have not been adequately investigated and are rarely considered in engineering practice. The seismic performance of structures when SSI effects are considered is still unclear, and the SSI concept is not devoid of misconceptions, particularly for RC wall-frame dual systems. The frequency response of the framework and its dynamic characteristics are heavily influenced by the simulation analysis of the soil beneath the foundations. The effect of SSI on geometry or plan irregularity is particularly highlighted in this study. The finite element software is used to complete the dynamic analysis of both the regular and irregular structures, and the SSI is also analyzed using the same software, SAP2000. The parameters drift, shear, time period, and frequency were prioritized for the dynamic analysis. The findings indicate that soil-structure interaction, particularly in soft soil cases, has a significant impact on the seismic response of Regular and Irregular buildings. The most significant increase in drift demands occurred in Irregular structures and the results for fixed-base, stiff, and moderate cases are more similar to each other than soft soil cases.

Electrocatalytic Reduction of 2-nitrophenol and 4-nitrophenol on Methyl Viologen Mediated IL platform

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ABSTRACT

In the present work, we report a Screen-printed carbon electrode (SPE) modified with redox mediated viologen ionic liquid (IL) over carbon nanotubes (MWCNTs) to notice the electrochemical detection of 2-nitrophenol and 4-nitrophenol for the first time. APMV was covalently connected with BMIM based COOH-IL through DCC coupling to form a stable amide linkage. Here APMV is used to endow electron transfer between MWCNT and electrode surface to enhance the sensitivity and the ionic liquids which is hydrophobic acts as a host for mediator immobilized as well as a binder. The synthesized COOH-IL was characterized using ^{1}H, ^{13}C NMR and FT-IR and HRMS. The electrochemical investigations were performed using cyclic voltammetry and the modified electrode exhibited two well-resolved redox peaks. The fabricated APMV-IL/MWCNTs/SPE showed a remarkable performance for electrochemical reduction of 2-nitophenol and 4-nitophenol. The proposed electrode further exhibited good stability and reproducibility.

Keywords: viologen, ionic liquids, 2-nitrophenol, 4-nitrophenol

The methylene blue dye degradation by using tungsten oxide with indium by a simple soft chemical route

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ABSTRACT

In this study, pure, indium-doped tungsten oxide (WO_3) nanoparticles were produced using a simple soft chemical technique at varying doping ratios between 0 and 3 at.%. Both pure WO_3 and WO_3 that has been doped with indium exhibit cubic crystalline structure, according to the XRD data. The surface morphology of the produced nanoparticles is seen in the SEM image. It has an longer irregular branched or network surface. Fourier Transform Infrared Spectroscopy (FTIR) investigation verified the existence of vibrational modes and elements. The photocatalytic activity of synthesised nanoparticles was measured. The efficiency of photocatalytic degradation was raised from 80% to 94%.

Key Words: Photocatalytic, Concurrently doped, Indium, Dye degradation, Methylene blue

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Cu(II), and Zn(II) Complexes Significantly Interact with Novel Pyridinehydrazones Discovered: Potential Cancer-Prevention Agents

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ABSTRACT

Introduction/Background: An estimated 9.6 million deaths, or one in every six deaths, were attributed to cancer in 2018, making it the second highest cause of death worldwide. To end cancer, novel and powerful chemotherapy is urgently required.
Methods: To determine the interactions between the synthesised Cu(II) and Zn(II) complexes and its pyridinehydrazone-based ligand, the structure of the complexes were studied.
Results: A new pyridinehydrazone-based ligand and its Cu(II) and Zn(II) complexes were synthesized. Structural characterization was done using elemental analysis, UV-Vis, FT-IR, ESI-MS, and NMR. The DFT calculations were used to determine the molecular structure of Cu(II) and Zn(II) complexes, which also supported the coordination geometry. The antiproliferative activity was tested against three cancer cells such as MCF-7 and MDA-MB-231 by MTT assay. The tests revealed that the compounds exhibited a higher antiproliferative activity than clinically used drugs.
Conclusions: The newly synthesized pyridinehydrazone and their Cu(II) and Zn(II) complexes showed excellent anticancer activity.

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A simulation study on the future green energy the nuclear energy through nuclear fusion

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ABSTRACT

Nuclear fusion has the potential to revolutionize future energy production. Unlike traditional energy sources, such as fossil fuels and nuclear fission, nuclear fusion produces no greenhouse gases or other harmful by-products. It also produces energy much more efficiently than other sources, making it a promising alternative for the future (1,2). The energy released during nuclear fusion can be converted into electricity through various methods, including steam turbines, thermoelectric generators, and magnetohydrodynamic generators. All these methods use the heat released during nuclear fusion to produce mechanical energy, which is then converted into electrical energy.

The current research work is a simulation study using Azore and Playgen software package, in developing the arc reactor to achieve controlled nuclear fusion. The software provides an efficient mechanism for controlling the reactor's energy output, a critical aspect of the system's safety.

The use of an arc reactor in combination with palladium core material to achieve controlled nuclear fusion is being investigated. To achieve this, Azore and Playgen software are proposed to be used to run a mechanism through the software for a more efficient process. In the first phase, deuterium and tritium isotopes of hydrogen are fused together in a reaction that released 17.6Mev energy.

The second phase is initiated as the energy released in the first phase fuses with palladium, producing a stable isotope of gold, a neutron, and additional energy. This reaction releases a tremendous amount of energy that is stored in the palladium core material surrounding the reactor. The fusion reaction in phase 2 produces 2.2 Mev energy.

This energy is then transferred to a heat exchanger, which converts the thermal energy into electrical energy.

Keywords: Nuclear fusion, Green energy, Deuterium, Tritium, Palladium

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Fluorescence chemosensor for fluoride ion using quinoline-derived probe: molecular logic gate application

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ABSTRACT

Here, we tested the existing cadmium probe (**P**) that could be used for the fluorescent detection of fluoride ions selectively over other anions. The strong emission was scrutinized at 500 nm for fluoride ions by **P** and concluded that it was caused by the hydrogen bonding interaction proceeded by deprotonation. As per Job's graph, the binding stoichiometric ratio between **P** and fluoride ion is 1:1 which has been confirmed by ^{1}H NMR titration, MS, and density functional theory studies (DFT). The detection limit for fluoride ion is 0.128 μM based on the concentration-reliant fluorescence titration. According to the findings, the probe is a strong contender for fluoride ion recognition. Further, **P** was also beneficial in the molecular logic gate and real water samples.

Selective colorimetric signaling of mercury (II) ions using a quinoline-based probe with INHIBIT logic gate behavior and test strip

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ABSTRACT

In this work, we studied the reported cyanide chromogenic probe (**L**) utilized to specifically detect Hg^{2+} ion using colorimetric technique. The addition of other metal ions had no impact on the colorimetric changes, which demonstrated that the probe could respond selectively to Hg^{2+} ion with clear color changes from yellow to orange. The binding mechanism of the probe towards Hg^{2+} ion is caused by the formation of a charge transfer complex with the lowest detection limit of 0.62 μM. The binding stoichiometry between the probe andHg^{2+} ion is 1:1 was confirmed by ^{1}H NMR titration, Job's plot, and FTIR analyses. It was observed that this chromogenic probe could be reversed with ethylenediaminetetraacetic acid (EDTA). This reversible chromogenic probe served as a fantastic tool for the molecular logic gate. The binding mechanism of the probe and Hg^{2+} ion was strongly validated by quantum mechanical analysis. This probe could also be used to assess the traces of Hg^{2+} ions present in water samples. Further, a test strip was also created by applying the probe on the filter paper face. Without the use of additional tools, this test paper facilitates the suitable recognition of the Hg^{2+} ion.

Green Synthesis and Characterization of Zinc Oxide Nanoparticles using Leaf Extract of Artemisia and their Antibacterial Applications

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ABSTRACT

The fabrication of plant-based nanoparticles has many benefits over conventional physico-chemical approaches and has multiple implications in biology and medicine. In the present study, a medicinal plant Artemisia pallens (*A. pallens*), was used to make zinc oxide (ZnO) nanoparticles (NPs) [1]. XRD, FTIR, SEM, and UV-Vis spectrophotometer were used to examine the structural and optical properties of NPs. The antibacterial activity of ZnO NPs was evaluated against various clinical strains such as *Staphylococcus aureus* (*S. aureus*), *Bacillus subtilis* (*B. subtilis*), *Escherichia coli* (*E. Coli*), *Pseudomonas aeruginosa* (*P. aeruginosa*), and fungi such as *Candida albicans* (*C. albicans*), *Aspergillus niger* (*A. niger*) [2]. UV peaks and XRD pattern matching that of JCPDS card for ZnO confirmed the presence of pure ZnO NPs. The existence of bioactive functional groups involved in the reduction of bulk zinc acetate to ZnO NPs is even further confirmed by FTIR. SEM images confirmed that the shape of NPs to be spherical [3]. The obtained ZnO NPs showed strong antimicrobial activity against clinical pathogens compared to conventional medications.

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Synthesis and Structural Analysis of pure Tin Oxide and Magnesium doped tin oxide Nano Particles

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ABSTRACT

The synthesis of pure Tin oxide and Magnesium doped tin oxide nano particles were carried out by co-precipitation method with EDTA as surfactant and sodium hydroxide as precipitator. Structure, size and surface morphology of pure and magnesium doped tin oxide were studied by X-Ray diffraction, The Powder XRD analysis showed sphere shaped tin oxide nano particles with chlorine contamination. The crystalline size determined by the Scherer formula was about 44nm. Lattice parameters were calculated and high quality of crystallization was determined. Doped Tin oxide is an oxygen deficient material which could be beneficial for transparent conducting oxide studies on structural properties of un doped and doped SnO_2.

SYNTHESIS AND CHARACTERIZATION OF ZINC DOPED ZIRCONIUM OXIDE NANOPARTICLES

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ABSTRACT

In the present work, undoped and zinc doped zirconium oxide nanoparticles with various weight percentage of zinc (0.04,0.08 and 0.12wt%) are synthesized by co-precipitation technique. The obtained nanoparticles are characterized by XRD and UV-VIS analysis. The XRD pattern shows that the pure ZrO_2 has stable tetragonal phase and also the zinc doped ZrO_2 shows tetragonal phase,this indicates that the Zn ion was well distributed in the host of the ZrO_2 matrix and the crystallite size also decreases with increasing zinc content. According to optical examination, the energy gap values decreased from 4.6eV to 3.4eV as Zn concentration increased

Zirconium oxide is a wide band-gap transition metal oxide with excellent mechanical, thermal, optical, and electrical characteristics. It can be widely used in the fabrication of structural ceramic devices, gas sensors, catalysts, and optoelectronic devices. Doping is an essential way to enhance the structural and optical properties of nanoparticles. The present study focusing on the synthesis of pure and zinc doped ZrO_2 nanoparticles by simple co-precipitation method and the obtained nanoparticles are characterized by XRD and UV analysis.

Pure and Zn doped zirconium oxide nanoparticles were synthesized from chloride aqueous solutions ($ZrOCl_2.8H_2O$, $ZnCl_2$) and NaOH act as precipitating agent. Aqueous solution of Zirconium oxy chloride and sodium hydroxide were taken in the ratio of 0.5:2. NaOH solution was added drop by drop till the pH value reaches 12 and stirred constantly for 2 hours at 60°C. Finally, the obtained precipitate slurry was filtered and washed with distilled water repeatedly and then finally with acetone to remove impurities. After drying, the obtained precursors were annealed at 500°C for 2 hours. Hereafter Zn-doped ZrO_2 nanoparticles were prepared, following the same procedure, for 0.04, 0.08 and 0.12wt% zinc concentration. The obtained products were characterized by X-ray diffraction analysis and UV analysis. X-Ray diffraction pattern of both pure and Zn doped ZrO_2 shows the tetragonal phase with high crystalline structure. Optical properties were studied using UV–Vis spectrometer and obtained band gap range between 4.6 and 3.4 eV.

Keywords: Zn doped ZrO_2, Co-precipitation.

Organoruthenium(II) complexes of phosphine–carboxamide based ligand: Structural diversities and catalysis perspectives

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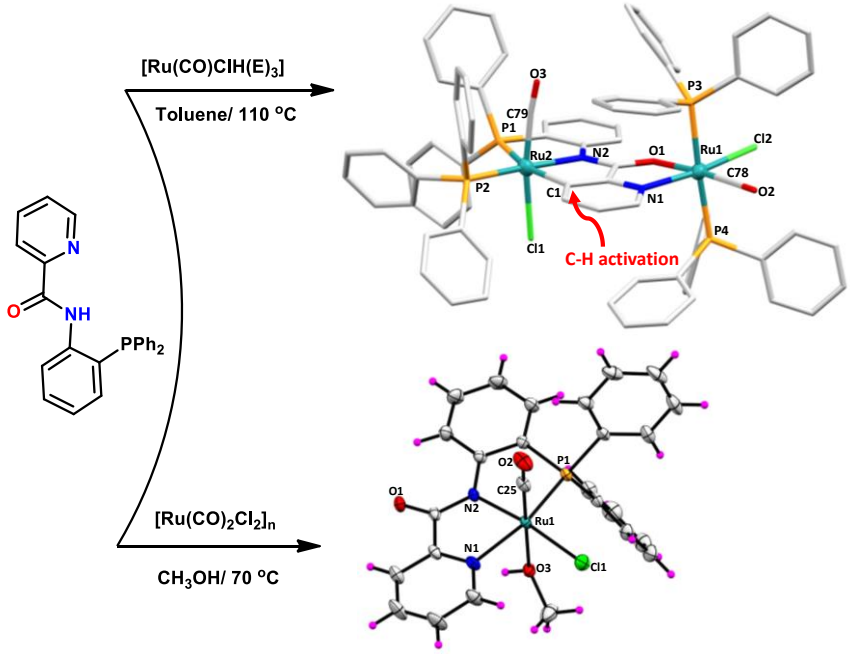
ABSTRACT

A new organo ruthenium(II) complexes bearing phosphine-carboxamide ligands, HL^1 (HL^1 = N-(2-(diphenylphosphanyl)phenyl)pyridine-1-carboxamide (HL^1) have been synthesized. These Ru(II) complexes have been characterized by using various spectroscopic techniques (FTIR, UV-Visible, ^1H, ^{13}C, ^{31}P-NMR and ESI-MS), conductivity and elemental analyses. The solid-state structures of Ru(II) complexes were substantiated by the single crystal X-ray diffraction technique that revealed versatile coordination modes of tridentate ligands varying between CNP and NO modes. All Ru(II) complexes exhibited a distorted octahedral geometry with a bidentate as well as tridentate ligand while other coordination sites are occupied by either anionic Cl^- or neutral co-ligands (CO, PPh_3). These well-defined ruthenium(II) complexes have been utilized as the homogeneous catalysts for the alkylation of amines using alcohols ensuing hydrogen borrowing strategy. The synthesized ruthenium(II) complexes were found highly active catalysts towards the N-alkylation of different amines with assorted alcohols and transfer hydrogenation of ketones.



Green Bricks from Brown Earth - A Review of Stabilized Mud Blocks for Energy-Efficient Buildings

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ABSTRACT

This paper provides a comprehensive review of stabilized mud blocks(SMB) as a sustainable alternative to traditional building materials. Although mud has been used as a building material for centuries, the addition of stabilizing agents such as cement, lime, and fly ash has significantly improved its strength and durability. These SMBs offer numerous advantages such as energy efficiency, affordability, and low carbon footprint. The paper discusses the various stabilizing agents, their effect on the properties of SMB, and the environmental impact of these blocks. Furthermore, the paper emphasizes the need for additional research on the long-term performance of SMB, as well as their potential for widespread adoption in the construction industry. The review concludes by highlighting the importance of additional research on the long-term performance of these SMBs, as well as their potential for wider adoption in the construction industry. Overall, the importance of sustainable building materials in mitigating the effects of climate change and achieving a more sustainable future is mentioned in this review.

Keywords: Stabilized mud blocks, low carbon footprint, energy efficiency, cement, lime, flash, climate change

Synthesis, Characterisation and Determination of antimicrobial, antioxidant, DNA binding and anticancer properties of the succinaldehyde based mannich base and its metal(II) complexes

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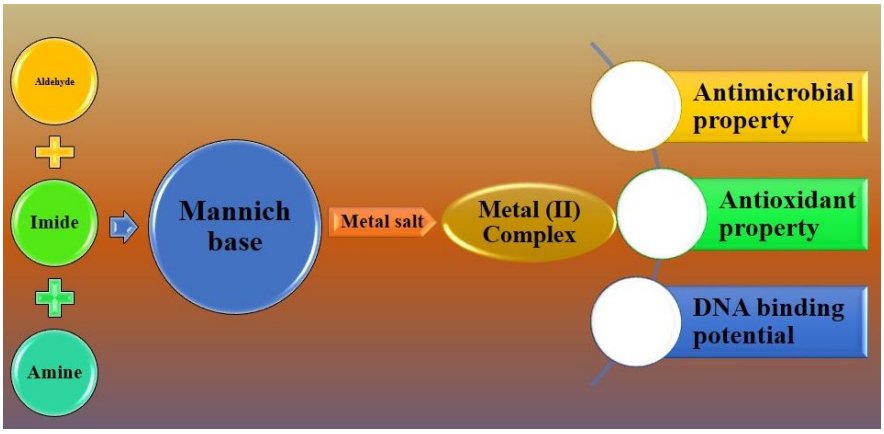
ABSTRACT

Succinaldehyde is an aldehyde well known for its antifungal, antibacterial, antiviral, and anticancer activities. It is also used as a cross linking agents for proteins. Maleimide is an imide with good anticancer properties. In the recent scientific era, a number of studies were made with these two compounds individually. In our current research work, we have prepared a new mannich base from maleimide, succinaldehyde and a known amine. The compound was characterized with UV-VIS, IR, NMR, ESR, and Mass data. Further to enhance the biological activity of the compound, it is coordinated with metals like copper and cobalt and the complexes are characterized separately. The test samples are analyzed for the antimicrobial properties against organisms like *Escherichia coli*, *Staphylococcus aureus*, *Aspergillus niger*, *and Candida albicans*, by agar-well diffusion method. The antioxidant potentials are studied with DPPH assay and reducing power assay. The extent of the ligand and the complexes to bind with DNA was determined from the results obtained from UV-VIS method and the fluorescence spectral analysis method.

Keywords: Mannich base; metal complexes; geometry; antioxidant property, DPPH, antimicrobial activity, DNA

Graphical ABSTRACT



A Critical Analysis on Future Lithium Ion Battery Technology with its Challenges and Risks Involved

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ABSTRACT

After Sony initially introduced lithium-ion batteries to the market in 1991, significant advancements in their performance have been realized. Because of its high energy density, low self-discharge, near-zero memory effect, high open circuit voltage, and extended lifespan, lithium-ion batteries (LIBs) continue to get a lot of interest as a viable energy storage technology. High-energy density lithium-ion batteries, in particular, have recently been regarded as the optimum power source for electric cars (EVs) and hybrid electric vehicles (HEVs) in the automotive industry. Although numerous unique technologies have been released to further increase LIB performance, some of them diverge significantly from the criteria. From this standpoint, certain new technologies are addressed in this paper such as Li-Air, Li-Metal, Solid State Lithium, Lithium Sulphur and many more. This paper compares the process, technology, benefits, risks and challenges involved. This paper also states the safety concerns and thermal problems of Lithium metallic combination batteries.

Keywords— Li-Air, Li-Metal, Li-Sulphur, Solid State Lithium, Electrolytes.

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Simple One-step synthesis of Gold Nanoparticles using Sparfloxacin for Ethanol Sensor Applications

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ABSTRACT

Alcohol is a dangerous substance that can cause a range of health problems and is a leading risk factor for death and disability globally. It also has a negative impact on mental health. Chronic drinking can lead to depression, anxiety, and cognitive decline. It is a major risk factor for the development of alcohol use disorders. The continuous monitoring and control of ethanol concentration in the human body can help to maintain the health. In this study, we have developed an electrochemical sensor for the non-invasive determination of ethanol concentration in human saliva. Initially, the gold chloride trihydrate (tetra chloroauric acid) was chemically reduced and stabilized by sparfloxacin (Sp) which resulted in the formation of gold nanoparticle (AuNPs). The formation of Sp-AuNPs was confirmed by utilization of FESEM, EDS, E-mapping, UV-vis and XRD. The synthesized stable Sp-AuNPs colloidal solution was used to modify the activated screen-printed electrode (Sp-AuNPs/A-SPE), which showed high sensitivity as well as selectivity towards ethanol (EtOH) oxidation in 0.1 M NaOH by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). The DPV technique used to determine the lowest concentration of EtOH from 25 µM to 350 µM, and the limit of detection (LOD) was 55 nM. The repeatability and reproducibility measurements were revealed that Sp-AuNPs/A-SPE are more stable and highly sensitive for in-situ determination of EtOH. As a result, our sensor system could be useful for highly sensitive and selective determination of ethanol. The use of Sp-AuNPs into ethanol sensors has the potential to get beyond some of the drawbacks of conventional sensors and bring ethanol sensing to a new level of accuracy and precision.

Keywords: Gold nanoparticles; sparfloxacin ; chemical synthesis; screen-printed electrode; ethanol sensor

Hemp derived cellulose based bionanocomposites for biomedical applications

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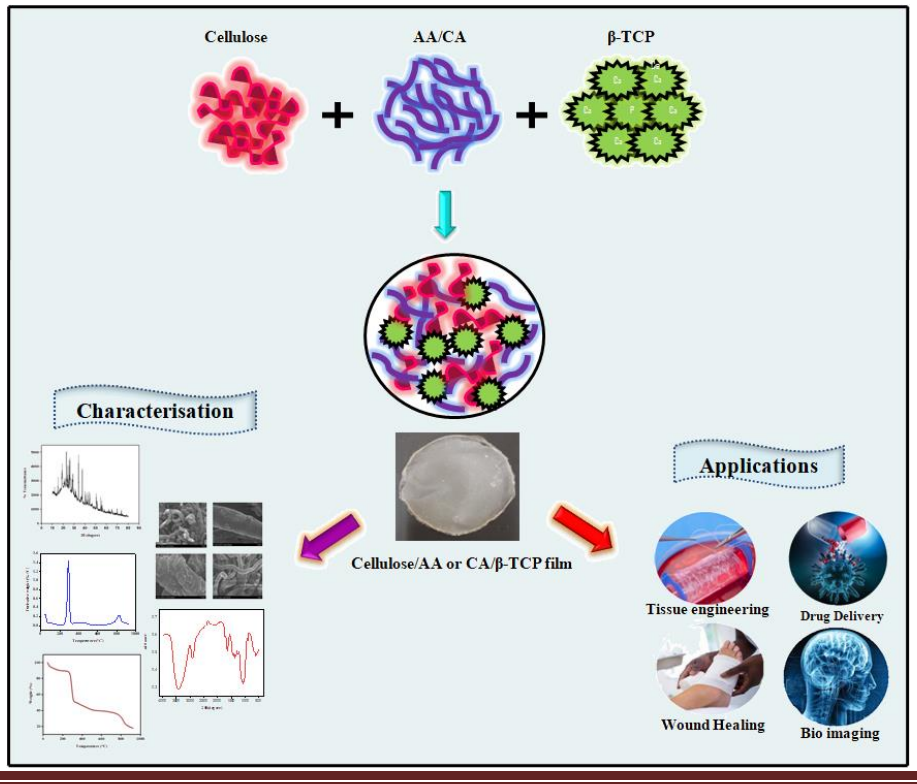
ABSTRACT

The composites made of biopolymers have been widely employed as promising materials for a variety of biomedical applications, including the fabrication of scaffolds and the transport of drugs, among others. As a result, researchers have concentrated their efforts on the development of innovative biomaterials to meet the need in the field of medicine. We present the synthesis and characterization of ceramic material incorporated triblock composite using cellulose isolated from hemp. The composites cellulose/Agar Agar (AA)/ β-tricalcium phosphate (β-TCP) and Cellulose/*I*-Carrageenan (CA)/ β-tricalcium phosphate (β-TCP) were prepared by solution casting method. The SEM images revealed that the addition of β-tricalcium phosphate results in significant morphological changes in the composites' surface and cross section. The thermal stability of the prepared materials was determined using thermal analysis. Also, the antimicrobial activities of the composite films such as antibacterial, antifungal, wound-healing, and anticancer properties were assessed and compared. The prepared bionanocomposites have the unique therapeutic value in a variety of biological applications.

Keywords: Biopolymer, cellulose, β-tricalcium phosphate, bionanocomposite, antimicrobial.

Graphical ABSTRACT



Biopolymer Composite Membrane for DMFC Application

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ABSTRACT

Direct Methanol Fuel Cell is one of the efficient, non-polluting, environmentally and economically advantageous energy conservation device. In the present study, Synthesized Surface modified zeolite (MZL) was introduced into the Chitosan matrix along with Halloysite Nano Tube (HNT) filler to prepare an eco-friendly biopolymer composite membrane for DMFC application. Structure of the prepared membrane was studied using XRD and FT-IR which confirms the fine dispersion of MZL and HNT in the Chitosan Matrix. Thermo gravimetric Analysis was done for the prepared membrane which confirms the membrane stability for the operating temperature of the DMFC. Electrochemical Impedance Spectroscopy study reveals the drastic improvement in the conductivity of the prepared bio composite membrane which is of the order of two magnitudes.

Key Words: Chitosan, Modified Zeolite, Halloysite Nano Tube, Proton Conductivity

Synthesis of Graphene mixed Bi_2S_3ZnO Nanocomposite and Efficient Environmental application for the Textile waste water Effluent under Sunlight Irradiation

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ABSTRACT

Environment friendly and efficient strategy for the preparation of Bi_2S_3ZnO–graphene(GR)based hybrid nanocomposite has been demonstrated by simple chemical approach for the photodegradation of Rhodamine B(Rh B)dye under solar irradiation. The resultant nanocomposite structure and composition has been characterized by Ultraviolet Diffusive Reflectance Spectroscopy (UV-DRS), Fourier Transform Infrared Spectroscopy(FTIR), Thermogravimetric Analysis (TGA), Raman spectroscopy and X-ray diffraction(XRD)studies. The incorporation of Bi_2S_3ZnO- graphene(GR) nanoparticles on the surface of GR was confirmed by High Resolution Transmission Electron Microscopy (HRTEM) and Field Emission Scanning Electron Microscopy (FESEM) studies. Electrochemical Impedance spectroscopy (EIS) and Cyclic voltammetry (CV) studies revealed that the incorporation of GR with Bi_2S_3ZnO nanoparticles significantly enhanced the redox property and electrical conductivity. During photocatalysis, the Bi_2S_3ZnO–GR nanocomposites have high photo catalytic activity compared with that of Bi_2S_3ZnO towards Rh B dye degradation under solar light irradiation. The enhanced photocatalytic activity might be attributed to the role GR played as an electron acceptor and transporter in the composite film, which effectively suppressed the charge recombination and promoted the charge transfer within the composite.

Keywords : Graphene, Bismuth, Rhodamine B, TEM, SEM, Nanocomposite

Facile synthesis of solid Zn-Doped Carbon Quantum Dots from Invasive *Prosopis Juliflora* plant for Photocatalytic and Antibacterial investigations

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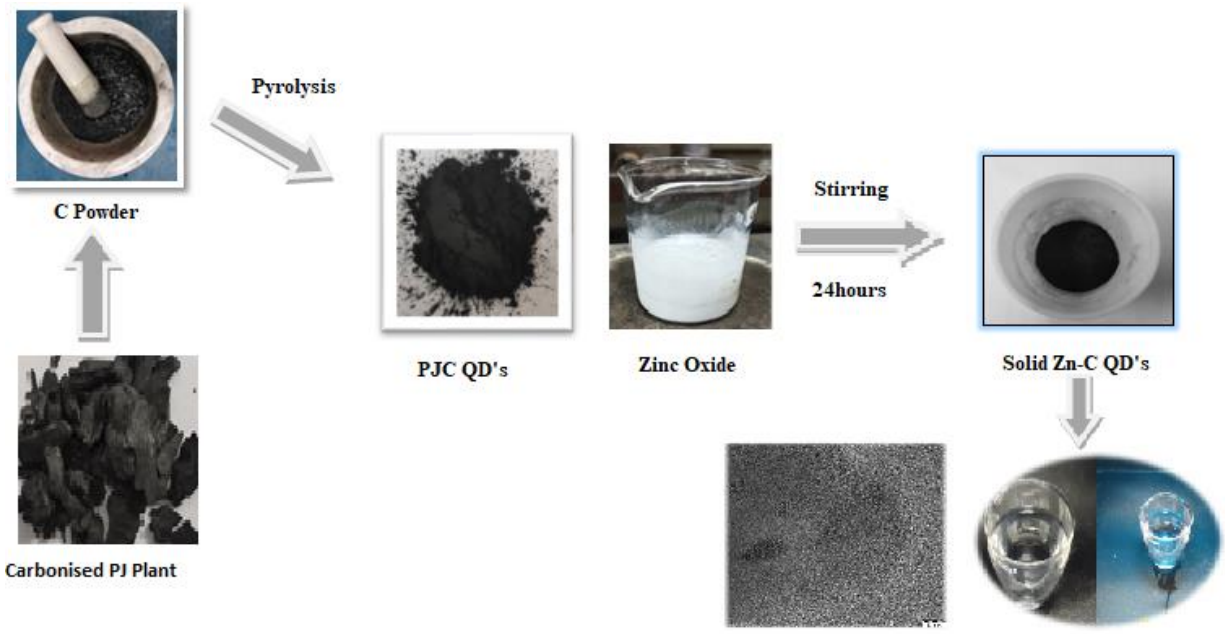
ABSTRACT

Carbon Quantum Dots (C-QD's) of high fluorescence and biocompatibility offers multimodal bio imaging applications, which has attracted substantial scientific attention. Here, we show a quick and easy two step approach to produce solid biocompatible Zn-C QD's using invasive *Prosopis Juliflora* plant as a precursor. The Functional groups of Zinc-Carbon Quantum Dot's (Zn-C QD's), OH, C=C, C-O-C and C-O are identified using FT-IR spectrometer (Nicolet 6700) 4000cm^{-1} to 400cm^{-1} with a resolution of 0.1cm^{-1}. Crystalline nature and morphology was analyzed by using X-ray diffractometer with Cu Kα radiation (λ = 1.54 Å) and Laser Confocal Raman spectrometer. High Resolution Transmission Electron Microscopy (HRTEM) images were attained using JEOL/JEM 2100 microscope in which lanthanum hexaboride (LaB6) was used a s electron source at an accelerating voltage of 200 kV and magnification of 2000-1500000 X. The synthesized Zn-C QD's shows excellent antibacterial and photocatalytic activity over PJC QD's.

KEYWORDS: *Prosopis Juliflora* Carbon Quantum Dots (PJC-QD's), Zinc-Carbon Quantum Dots (Zn-C QD's), pyrolysis.



Hydrothermal synthesis of visible light active C3N4 modified Bi_2WO_6 nanocomposites and its photocatalytic activity

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ABSTRACT

Bi_2WO_6 is a layered semiconductor have excellent photocatalytic property against organic dyes. Though materials like TiO_2 are believed to possess excellent photocatalytic activity, its inability to absorb visible light limits its application. In this current work, Bi_2WO_6/C_3N_4 nanocomposites were prepared by two step method. C_3N_4 and S-C_3N_4 obtained by thermal polymerization of melamine was used during the hydrothermal synthesis of Bi_2WO_6 to get the desired composites. The synthesized composites were characterised by various techniques like powder X-ray diffraction (XRD), UV-Vis spectroscopy, Fourier transform infra-red spectroscopy (FTIR), field emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM). In addition to its photocatalytic performance, effect of catalyst dosage, pH, concentration of dyes, etc. are studied. The nanocomposite thus prepared, can be an asset for the researchers working in the area for photocatalysis.

Bioactive composite coating on metal surface using Electrophoretic deposition method (EPD)

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ABSTRACT

Coatings and bioactive composite play a key role in recent years for orthopedic implants. To overcome corrosion and also to enhance bioactivity of the substrate, surface modification using functionalized bioactive composite coating is a viable option. Electrophoretic deposition (EPD) has a promising technique to achieve a adhesive coating on metal surface and it also provides a fine, uniform & strong coating among all other coating techniques. A bioactive composite coatings (n-HAP, GO) were used to enhance the mechanical properties of the bio implant. Change in coating voltages and time is used to optimize a fine coating on metal surface. The coated samples were optimized in various sintering temperature to analyze the surface strength. After that, all the coated samples were tested with basic characterization techniques like XRD, FTIR and Optical microscope images to measure the coating thickness. To enhance the corrosion behavior, the coated samples were allowed in a corrosion medium for testing using electrochemical parameters. Evaluated bio implants were used for bone implant applications in orthopedic surgeries.

Key words: Electrophoretic deposition, Corrosion, Bioactive composite, Coatings

DESIGN AND ANALYSIS OF BLENDED WING AND MIDDLE WING AIRCRAFT

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ABSTRACT

When Aircraft or any automobile vehicles moving in the fluid medium it can face drag. Many researches are going to reduced drag but drag can't totally eliminated in the moving object. In this project we have analyzed the different wing and found the co-efficient of lift and co-efficient of drag and lift per drag ratio. The middle and Blended wing are simulated in computational fluid dynamics software. And then the geometries designed by using Catia and ICEM CFD. The purpose of the analysis is to find the maximum lift location of wing and minimum drag location of the wing especially in blended and middle wing. A BWB configuration has a superior in-flight performance due to higher l/d ratio and could improve upon existing conventional aircraft in the area of noise emission, fuel consumption and direct operation cost on surveys. BWB configuration needs to employ a new structural system for passenger safety procedures such as passenger ingress. The beneficial results of the BWB design were that the parasite drag was decreased and span wise body as a own whole can generate lift. In this research conceptual BWB designs and CFD simulations were iterated to evaluate the aerodynamic performance of an optimum BWB design and theoretical calculations of structural analysis was done based on CFD results.

DESIGN AND ANALYSIS OF GAS TURBINE COMBUSTORS

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ABSTRACT

Gas turbine engines have the most advantages in the power generation on many aircrafts and the combustion chamber in the aero engines plays the major role of it. This project explains designing and modeling and analyzing of the annular combustion of the gas turbine engine. As we know combustor is the heart of any engine, where incoming pressurized air is heated by burning of hydrocarbons. A combustor of gas turbine should be compact simple, long operative and robust in construction. This is capable of sustaining variables in fuel flow rate. The material selection and flame stabilization. Precaution have been taken. Design is economically assembly is made also less complicated to analyze and project is completed in minimum duration. The specialty of the project is to is to study the design difficulties of combustor and flow examination with the help of CFD application. The swirl vanes are designed in such a manner that flow turns at 30° from the previous path. This combustor has provision for flame tube cooling also, one row of holes on both the inner and outer domes is made parallel to the axis of the combustor compared to the other rows of holes, which are at 30°.The exit of the combustor has number of stator blades to re-direct the flow to the blades.

Synthesis and Optical Characterization of Silver Doped Hydroxyapatite and It's Antimicrobial Activity

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ABSTRACT

The synthesis of nanosized particles of silver doped hydroxyapatite with antibacterial properties is of great interest for the development of new biomedical applications. In this work silver doped nano hydroxyapatite was bio-synthesized. A silver-doped nano hydroxyapatite was synthesized at 100°C in deionised water. Further, the synthesized silver doped hydroxyapatite nanoparticles are evaluated for their antimicrobial activity against Gram-positive and Gram-negative bacteria and fungal strains. Optical spectroscopic characterization of the final nanoparticles was carried out using UV-Visible spectrometer. From the UV-visible spectroscopic technique absorption region was noted. The structural characterizations were carried out with XRD and SEM techniques. The XRD also used to calculate the particle size of the silver hydroxyhapaitate (Ag-HAP) nanoparticles (NPs).

Key words: silver nanoparticle, hydroxyapatite, antibacterial activity

Nitrogen-rich graphitic carbon nitride (g-C_3N_5)-based nanostructures for energy and environmental applications

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ABSTRACT

The rapid development of the global population has considerably increased energy depletion and stress on the environment. Hence, new functional materials with fascinating properties offer opportunities to address these issues. In this regard, graphitic carbon nitride (C_xN_y) family, especially the nitrogen-rich graphitic carbon nitride (g-C_3N_5) has received much attention due to its easy of synthesis, metal-free organic nature, and tuneable energy gap. g-C_3N_5 has been broadly used for energy conversion applications (water splitting) and environmental dye degradation. The band gap is important for electrochemical energy conversion and environmental dye degradation. Generally, the band gap of the g-C_3N_4 lies between 1.76 - 2.2 eV. It is essential to tune the energy gap of the g-C_3N_4 based on the end application. The physical and chemical properties such as band gap, structural defect, vacancy creation and morphology of g-C_3N_4 are tuned by various strategies including different synthesis approaches, elemental doping, composite formation, and construction of heterojunction. Remarkable studies on (g-C_3N_5)-based nanostructures have been witnessed in the past few years. However, there are still some challenges and issues to be attempted.

Keywords: *graphitic carbon nitride, g-C_3N_5, band gap, energy conversion applications, environmental remediation.*

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HIGHLY VISIBLE LIGHT DRIVEN $Ce_2(MoO_4)_3$) /ZnO NANOCOMPOSITE FOR EFFECTIVE REMOVAL OF AQUEOUS ACID GREEN-16 DYE

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ABSTRACT

In this research work, we used the hydrothermal technique to create an $Ce_2(MoO_4)_3$) /ZnO nano heterojunction photo catalyst. A variety of techniques were used to characterize the prepared photo catalyst, including Fourier transform infrared analysis (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX) with elemental colour mapping (ECM), high-resolution transmission electron microscopy (HR-TEM) with, UV diffuse reflection. The degradation of Acid Green was studied using $Ce_2(MoO_4)_3$/ZnO nano heterojunctions photo catalytic activity under UV light. In neutral pH, it has been discovered that Ce2(MoO4)3) /ZnO is more efficient than prepared ZnO at mineralizing Acid Green. The photo catalyst's stability and reusability were also identified. The technique was shown to be successful in the industrial effluent after the influence of common ions on degrading efficiency was investigated.

Keywords: Photo degradation, Ce2(MoO4)3), Wastewater Treatment, Acid Green, hydrothermal Technique

A Novel Hybrid Technique to Predict Solar Radiation Using Support Vector Machine and Search Optimization Algorithms

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Abstract

The use of intelligent algorithms for global solar forecasts is a great tool for studying solar energy use. Solar radiation forecasting is helpful in places lacking meteorological stations for a number of energy-generating and transportation applications. Throughout history, many methods of estimating solar radiation, such as neural networks (ANN) or machine learning (ML), have been utilized, with ML being the most prominent. The support vector machine is a machine learning (ML) classification system used to anticipate solar radiation (SVM). Search optimization algorithms (SOA) such as genetic algorithms (GA) and particle swarm optimization algorithms (PSO) were employed to increase prediction accuracy. This study examines several hybrid SVM models with SOA to determine the best settings for lowering the forecast error of solar radiation using meteorological data. We looked at research publications from the previous five years on forecasting solar radiation using SVM models and hybrid SMV-optimized models with SOA. The results show that SVM with GA outperforms typical SVM models that use the Radial basis kernel function for prediction parameters.

Keywords: Solar radiation, Support Vector Machine (SVM), Renewable energy, and Solar energy systems.

EXPERIMENTAL INVESTIGATION ON STRENGTH AND DURABILITY OF SELFHEALING CONCRETE USING BACTERIA AND MINERAL ADMIXTURES

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ABSTRACT

Experimental investigation on this study is to evaluate the mechanical and durability properties of self-healing strength of concrete specimen by incorporating an alternative for cement along with mineral admixture, along with Bacteria for Healing cracks. The classic method which are used for healing cracks involves the use of ordinary synthetic polymers which causes a lot of damage to the environment .Therefore, The use of sustainable strategies like ingesting bacterial culture and mineral admixture into the concrete mix along with an alternative replacement of cement can act as an active support for both nature as well as construction industries.in this Abstract, control concrete, concrete made by replacing cement with as mineral admixture bacteria induced concrete and compared. The bacteria mixed in control as well as mineral admixture made concrete specimens at different levels for each different specimen. Characteristic compressive strength of self -healing concrete has been identified for various age of specimen. Cylinder and Beams are compared on ground of Compressive strength, Split tensile strength, Flexural strength, Water absorption and Sorpitivity. Further, an artificial cracks was induced in the specimen and the bacterial healing activities along with calcite precipitation where examined through Scanning Electron Microscope (SEM) and Visualized Analysis

Keywords *— Mineral admixture, Bacteria, Self -healing concrete, Compressive strength, Mechanical and Durability properties.*

Antioxidant, antimicrobial, DNA binding studies of Cu (II) complex of Nicotinamide based Mannich base ligand

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ABSTRACT

New novel research work, synthesis of biologically active Cu(II) complex from nicotinamide based Mannich base ligand. The synthesized ligand and its Cu(II) complex was characterized by elemental analysis, electronic absorption, FT-IR, ESR and mass spectrometric methods. The results show that Cu(II) complex has square planar geometry. Antioxidant and antimicrobial results show that Cu(II) complex has good radical scavenging and antimicrobial activity than prepared ligand. Furthermore, DNA and BSA binding activities of Cu(II) complex has been studied by electronic absorption and fluorescence techniques. The result suggests that Cu(II) complex successfully interact with DNA and BSA molecules.

Keywords: Mannich base; Cu(II) complex; antioxidant; DNA binding; BSA binding

Antioxidant, antimicrobial, DNA binding studies of Ni(II) complex of Nicotinamide based Mannich base ligand

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ABSTRACT

In this present research work, synthesis of biologically active Ni(II) complex from nicotinamide based Mannich base ligand. The synthesized ligand and its Ni(II) complex was characterized by elemental analysis, electronic absorption, FT-IR. The results show that Ni(II) complex has square planar geometry. Antioxidant and antimicrobial results show that Ni(II) complex has good radical scavenging and antimicrobial activity than prepared ligand. Furthermore, DNA binding activities of Ni(II) complex has been studied by electronic absorption and fluorescence techniques. The result suggests that Ni(II) complex successfully interact with DNA molecule.

Keywords: Mannich base; Ni(II) complex; antioxidant; Antimicrobial;DNA binding

Antioxidant, antimicrobial, DNA binding studies of Co (II) complex of Nicotinamide based Mannich base ligand

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ABSTRACT

In this research work, synthesis of biologically active Co(II) complex from nicotinamide based Mannich base ligand. The synthesized ligand and its Co(II) complex was characterized by elemental analysis, electronic absorption, FT-IR, ESR and mass spectrometric methods. The results show that Co(II) complex has square planar geometry. Antioxidant and antimicrobial results show that Co(II) complex has good radical scavenging and antimicrobial activity than prepared ligand. Furthermore, DNA and BSA binding activities of Co(II) complex has been studied by electronic absorption and fluorescence techniques. The result suggests that Co(II) complex successfully interact with DNA and BSA molecules.

Keywords: Mannich base; Co(II) complex; Antimicrobial ;Antioxidant; DNA binding.

Antioxidant, antimicrobial, DNA binding studies of Zn(II) complex of Nicotinamide based Mannich base ligand

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ABSTRACT

In this research work, synthesis of biologically active Zn(II) complex from nicotinamide based Mannich base ligand. The synthesized ligand and its Zn(II) complex was characterized by elemental analysis, electronic absorption, FT-IR, and NMR spectrometric methods. The results show that Zn(II) complex has square planar geometry. Antioxidant and antimicrobial results show that Zn(II) complex has good radical scavenging and antimicrobial activity than prepared ligand. Furthermore, DNA binding activities of Zn(II) complex has been studied by electronic absorption and fluorescence techniques. The result suggests that Zn(II) complex successfully interact with DNA molecule

Keywords: Mannich base; Zn(II) complex; Antimicrobial ; antioxidant; DNA binding; BSA binding

Synthesis, Characterization, types and Application of Nanoparticle

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ABSTRACT

In the present study the silver nanoparticles was prepared by using chemical synthesis. The nanoparticles of Silver nanocolloid solution has been prepared chemically by the reduction of silver salt using nano material. The nanoparticles were also prepared by reducing silver salt using ascorbic acid which is a mild reducing agent. The nano particles preparation a, types and properties was discussed the nanoparticles were also characterized by UV-VIS spectroscopy and scanning electron microscopy (SEM).

Keywords:
Nanoparticles , Types, Properties , Application Characterization.

Synthesis and Characterization of Silver Nanoparticle by Chemical reduction method ($NaBH_4$)

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ABSTRACT

In the present study the silver nanoparticles (Ag-NPs) were prepared by using chemical synthesis. The Silver nanocolloid solution has been prepared chemically by the reduction of silver salt using sodium borohydride ($NaBH_4$). Triangular silver nanoparticles were also prepared by reducing silver salt using ascorbic acid which is a mild reducing agent. The nanoparticles were also characterized by UV-VIS spectroscopy and scanning electron microscopy (SEM).

Keywords: Silver nanoparticles (Ag-NPs), ascorbic acid, reducing agent, SEM.

Isolation and Characterization of Andrographolide from *Andrographis paniculata* and its *Invitro* Antidiabetic Activity

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Andrographis paniculata (Acanthaceae), is widely used in Indian systems of medicine as a stomachic, tonic, antipyretic, alterative, anthelmintic, febrifuge and cholagogue; for liver disorders, general debility and colic pains. The leaf forms an ingredient of many patented Indian herbal proprietary preparations for the treatment of liver ailments. In this work, a simple and rapid method for isolation of andrographolide from the leaves of *Andrographis paniculata* is reported. This involves extraction of the leaf powder by cold maceration in a 1:1 mixture of dichloromethane and methanol and isolation of andrographolide directly from the resulting extract by recrystallisation. The identity of the compound was confirmed through IR, ^{13}C NMR, ^{1}H NMR. Further, the isolated compound was studied for alpha (α)-amylase and alpha (α)-glucosidase inhibition using an in vitro antidiabetic model, exhibited significant α-amylase and α-glucosidase inhibitory activities with an IC_{50} value of 31.5 µg/mL and 79.51 µg/mL respectively and well compared with standard acarbose drug.

Green synthesis and electrical properties of AgO nanoparticles using leaves of *Anisomeles Malabarica*

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ABSTRACT

Semiconductor nanoparticles are of great interest both for fundamental research and technological applications as a consequence of the large ratio of surface to volume atoms and quantum confinement of the excitons. Recently, the synthesis of inorganic nanocrystals has attracted much interest due to their strong size dependent, special optical, electronic properties and potential applications in electronics, optics and catalysis. Particularly, metal nanoparticles are more frequently used in "green synthesis" due to their peculiar chemical, photo-chemical, and electrical properties. In the present work, synthesis of AgO nanoparticles using leaves of *Anisomeles Malabarica* were successfully prepared by the microwave assisted solvothermal method. Powder X-ray diffraction studies showed that the biosynthesized AgO NPs were crystalline in nature. The FTIR analysis confirms the presence of various functional groups in the leaf extract as well as in the NPs. The electrical properties of AgO nanoparticles have been studied by dielectric and also ac conductivity measurements. The results suggest that it may be used as microelectronic applications.

Keywords: Nanoparticles; Green Synthesis; Electrical; Dielectric; Conductivity

Biological properties of ZnO Nanoparticles Using Leaf Extract of *Anisomeles Malabarica*

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ABSTRACT

Green synthesis has been considered as another remedy in the field of medicine. Aside toxic chemical and physical method, biological method is considered using medicinal plants extract were used for the synthesis of nanoparticles. The surface and fraction of the atoms are responsible for the activity of the nanoparticles. This invention of green nanotechnology is considered ecofriendly and cost effective when compared to the others. The technology utilizes proteins as natural capping agents and its synthesis from plants utilize various secondary metabolites, enzymes, proteins and or other reducing agents which makes it suitable to use in various biomedical and clinical applications. In the present work, investigation on the anti-bacterial and anti-arthiritic activities of ZnO NPs prepared by using *Anisomeles Malabarica* leaf extract is made and succeeded. The preparation of ZnO nanoparticles (NPs) was investigated in relation to experimental factors such extract concentration, temperature and pH. The antibacterial properties of synthesized ZnO NPs were investigated and developed as antibacterial agents against a wide range of Gram-positive and Gram-negative bacteria to control and prevent the spreading of bacterial infections. Protein denaturation and proteinase inhibitory activity of produced ZnO NPs were investigated for antiarthritic activity. The synthesised ZnO NPs in the current study are a potential candidate for a number of biological activities, and as a consequence, they can be helpful to the medical sector, according to all the results.

Keywords: Nanoparticles; Green Synthesis; Antiarthritic; ZnO;

Zinc Oxide Nanoparticles Biosynthesis using *Azadirachta indica* (Neem) Leaf Extracts and their Potential as Antimicrobial Agents

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ABSTRACT

Nanoparticles have attracted considerable interest in isolated and in consolidated forms as they exhibit unique properties that differ significantly from their coarse-grained counterparts. Metal nanoparticles have many potential applications, including use in biomedical, optoelectronic and catalysis systems which relate to their size-dependent properties. The properties of materials prepared by different methods are critically dependent on the nature of preparation technique and subsequent heat treatments like annealing in air, vacuum or different gaseous environments like H_2, N_2, Ar. etc. In the present work, *Azadirachta indica* (Neem) leaves were used in a simple domestic microwave-assisted solvothermal synthesis process to produce zinc oxide (ZnO) nanoparticles (NPs). The study is to focus at the evaluation of the potential of the antibacterial activity of the synthesized Zinc oxide nanoparticle using *Azadirachta indica* leaf extracts on selected bacterial; E.coli, S. aureus, K. pneumonia. Zinc oxide (ZnO) nanoparticles synthesized, spectral and optical studies were used to characterize the nanoparticles. The particles were further subjected to evaluation of their activity. This study being the first using *Azadirachta indica* leaf extract should provide a new agent toward the fight of resistance bacterial and effective therapies in the field of medicine.

Keywords: Nanoparticles; Green Synthesis; Antimicrobial; Spectral; Optical

Spectroscopic Investigations on NLO Single Crystals of Manganese Mercury Thiocyanate

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ABSTRACT

The organometallic complexes of thiocyanate are desirable nonlinear optical materials for realizing blue-violet light by frequency doubling of laser radiation. The experiments conducted by Chinese and Indian research groups strongly favour the possible use of this class of materials for various nonlinear optical applications and photonics device fabrications. In the case of Manganese mercury thiocyanate (MMTC), bulk size crystal was successfully achieved by slow cooling method. Though single crystals were obtained by the conventional slow evaporation method, the harvested size of the crystal was not encouraging. The growth of MMTC by vertical Bridgman configuration proved to be a useful one but the presence of inclusions and clustering of the crystals remains as a minor concern. Single crystal X-ray diffraction (XRD) data reveals that the grown crystals belong to the teteragonal system with $I\bar{4}$ space group. The crystals are characterized using optical absorption, Fourier transform infrared (FT-IR), energy dispersive X-ray analysis (EDAX) studies. The second harmonic generation (SHG) efficiencies of the grown crystals are also measured using Kurtz and Perry powder technique.

Keywords: Organometallic; Growth; Optical; Single crystal; SHG

Growth and charecterization of Zinc cadmium thiocyanate (ZCTC) single crystals for optoelectronic applications synthesized by SR method

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ABSTRACT

Second order nonlinear optical (SONLO) materials capable of frequency conversion into visible and ultraviolet (UV) wavelengths are intensively studied for the past 50 years. Such materials are widely used in device fabrications relating to telecommunications, optical computing, optical disk storage and optical information processing. Hence, it is of vital importance to find out the linear as well as nonlinear optical properties of the developed samples. In the current study, X-ray diffraction, FTIR, UV-visible, and etching were used to successfully analyze the synthesis of zinc cadmium thiocyanate (ZCTC) and the irradiation effect. Temperature and frequency effects on the crystal's dielectric response were investigated. According to dielecrtic research, the dielectric constant and dielectric loss at all frequencies drop as the temperature rises.

Keywords: NLO, Organometallic, Dielectric, Irradiation

PERFORMANCE EVALUATION OF SULFONATED POLYSULFONE - SBA 15 ELECTROLYTE MEMBRANES FOR FUEL CELL

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ABSTRACT

The prepared mesoporous SBA-15 (Santa Barbara Amorphous-15) was sulfonated and used as filler for the preparation of sulfonated polysulfone based composite electrolyte membranes. The SBA-15 and polysulfone were sulfonated using sulfonating agents like 3-mercaptopropyl trimethoxysilane and trimethylsilyl chlorosulfonate, respectively. The different weight percentages (1, 3, and 5 wt %) of sulfonated SBA-15 (SSBA-15) were used to prepare composite electrolyte membranes. Membrane properties like water uptake, ion exchange capacity, swelling ratio, and proton conductivity of the composite membranes were studied for assessing the suitability of the electrolyte membranes for use in fuel cells. Characterization techniques such as FT-IR, XRD, SEM, TEM, and BET were used to study the physico-chemical properties of the electrolyte membranes. TEM and BET analysis showed that SBA -15 retained its mesoporous structure even after the sulfonation process. The prepared membranes were then tested in an in-house built single-cell fuel cell using hydrogen as fuel and oxygen as the oxidant. The fuel cell study showed that the presence of Sulfonated SBA-15 in the polymer matrix provided additional ion exchange sites and retained water for proton transfer which resulted in higher power density of 815 mW/cm^2 with SPSU + 3%SSBA-15 membrane as compared with Nafion 117®.

Keywords: Sulfonation, SBA – 15, Polysulfone, Electrolyte, PEMFC.

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Optimized Biodiesel Production from Hibiscus Cannabinus seed oil using Barium Oxide (BaO) Nano-catalyst

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ABSTRACT

Biodiesel production from Hibiscus cannabinus seed oil provides an alternative energy means of producing liquid fuels from biomass for various uses. Biodiesel production by bio-oil and methanol in the presence of Barium oxide (BaO) nano-catalyst offers several benefits such as environmental, waste management and economically. A nano-catalyst of BaO was synthesized by thermal-decomposition method and calcinated at 450 °C followed by characterization using SEM, TGA, XRD, and FTIR techniques. The maximum conversion of Bio-oil to biodiesel was estimated to be 94%, at optimized experimental conditions, 60 °C, and 1:10 Bio-oil oil to methanol ratio, 1.5% by weight of catalyst loading rate and 110 minutes reaction time, which is among few maximum conversions resulted so far. Biodiesel parameter were analysised according to the American (ASTM D6571) fuel standards. All reactions are carried-out under atmospheric pressure and 1450 rpm of agitation.

Keywords: Biodiesel; BaO Nano- catalyst; Thermal- decomposition.

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Influence of Ag/V Co-Doped Hydroxyapatite and its antimicrobial activity

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ABSTRACT

As hydroxyapatite resembles human bone, it has been received the most attention as a biomaterial for use in bone transplants, scaffolds, fillers, cements, coatings, and other procedures to repair and regenerate bone defects. For a tissue engineering scaffold, it is essential to create bone grafts and scaffolds with the appropriate interconnected porosity and adequate strength. Hydroxyapatite is a naturally or synthetically occurring compound. It majorly consists of calcium and phosphate. Doping is one of the effective strategies to improve the strength of the material. The aim of this study was to synthesis pure hydroxyapatite [$Ca_{10}(PO_4)_6(OH)_2$] and Silver (Ag)/Vanadium(V) co-doped hydroxyapatite [$Ca_{10-x}Ag_x(PO_4)_{6-x}(VO_4)_x(OH)_2$] with various concentration such as (x= 0.01, 0.05, 0.1M). Pure Hydroxyapatite and the Silver and Vanadium doped Hydroxyapatite have been synthesized using the chemical precipitation method. Ag^+ and V^{+5} ions replace Ca^{2+} and PO_4^{3-} in hydroxyapatite, respectively. The synthesized samples were characterized using X-ray diffraction (XRD), Fourier transform infrared (FTIR), Field emission scanning electron microscope (FE-SEM), Energy dispersive x-ray analysis (EDX). The antibacterial activity pure and co-doped Hydroxyapatite were investigated.

Eco-friendly Synthesis of Silver Nanoparticles using *Ocimum sanctum* Leaf Extract

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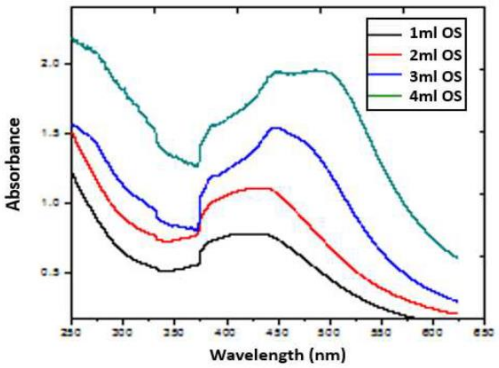
ABSTRACT

Nanoparticles are vital part in a wide range of utilizations, including medication, semiconductors, catalysis and energy. The most tough stage in the field of nanotechnology is producing nanoparticles in a reliable, environmentally friendly, cost-effective, and efficient manner. Green synthesis of nanoparticles using plant-derived materials is highly regarded in comparison to all other synthesis routines due to its low toxicity, eco-friendliness, and high efficiency. The current study describes a simple, effective, and environmentally friendly method for producing silver nanoparticles using *Ocimum sanctum* L. leaf extract. In addition, we prepared *Ocimum sanctum* L. leaf extract using the much more environmentally friendly ultrasonication extraction technique. UV-Visible spectroscopy was used to characterize the synthesized silver nanoparticles. UV-Visible spectroscopy results revealed the absorption bands in the range of 423-492 nm, confirming the formation of the silver nanoparticles.

Colour Change during the formation of silver nanoparticles at varying volume of *Ocimum sanctum* leaf extract



UV-Visible spectrum of Ag nanoparticles at varying volume of leaf extract

Keywords: Eco-friendly, *Ocimum sanctum*, silver nanoparticle, ultrasonication

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Effect of physical, chemical, biological and binding properties of 2-bromo-3,3,5-triphenyl-2,3-dihydrofuran green solvents by DPT and TD-DFT approach: an antiviral agent

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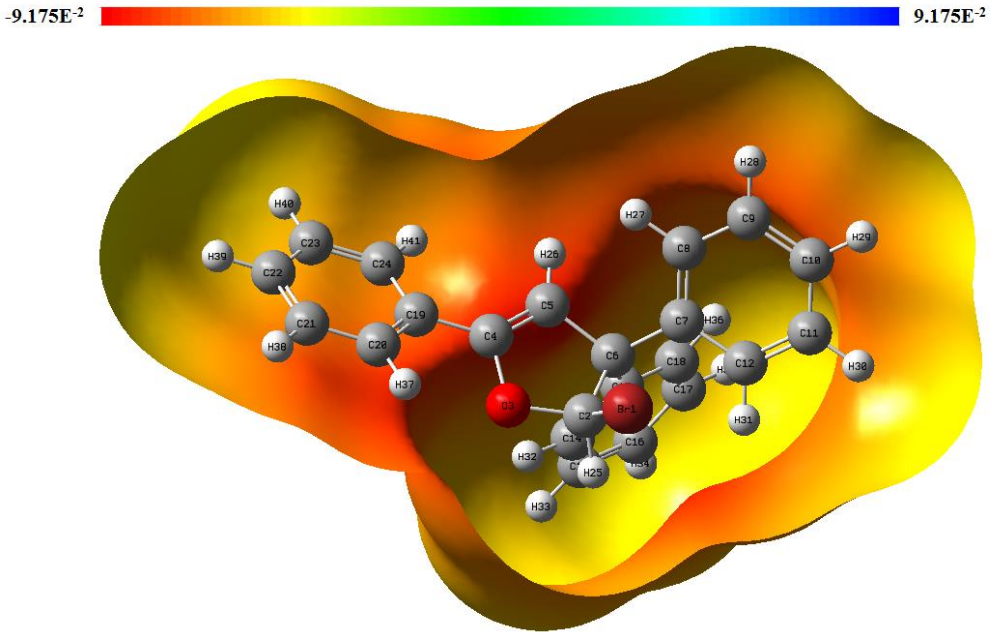
ABSTRACT

Density functional theory (DFT) is applied to 2-bromo-3,3,5-triphenyl-2,3-dihydrofuran (2BTPDF). B3LYP technique and 6–311++G(d,p) basis set are used to determine the optimal structure and different physical, chemical and biological properties. Bond energies and ellipticity are determined using atoms in theory of molecules (AIM). NBO analysis is used to study the exchanges between the contributor and the recipient through energy. By using the HOMO-LUMO values and critical electronic parameters, the stability is determined. The molecular electrostatic potential (MEP) and the Fukui function from Mulligan charges are used to determine the reactive parts of the molecule. The TD-DFT technique obtains the electronic transition using the UV-Vis spectrum with various solvents. NLO studies were performed on this molecule. Studies of temperature effect on 2BTPDF are performed using thermodynamic parameters. Drug modeling and molecular docking tests are used to evaluate biological activity and antiviral properties.

Keywords: DFT, MEP, NLO, Fukui function UV–Vis Docking

Graphical abstract



Solvent polarity, structural and electronic properties in various solvents and biological studies of 3,3,5-triphenyl-2,3-dihydrofuran-2-ol carcinogens in blood cells

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ABSTRACT

The present work involves the synthesis, characterization and computational evaluation of 3,3,5-triphenyl-2,3-dihydrofuran-2-ol with density functional theory (DFT) as the underlying principle. The theoretical optimum structure and corresponding geometrical parameters were obtained. Multiwfn 3.8 was used to perform topological studies such as R D G, E LF, L O L, and charge transfer analysis used to identify excited states, non-covalent interactions, and critical bonding regions in the molecule. Since furanones interact with more polar solvents, the effect of solvents on the variation of molecular properties with different polar solvents was studied with the IEFPCM model. Solution studies have been shown to influence FMO, UV, MEP and NLO analyses, and therefore, between the gas and solvent phases, variation is observed in the properties under study. NBO probes were analyzed to identify the natural bonding orbitals within the molecule that contribute most to the stabilization energy of the title compound. Pharmacological evaluation was performed using readily available online tools including SwissADME, Pre-ADMET, GUSAR and ADMETLab 2.0 to determine the medicinal chemical properties of the molecule. Also, molecular docking of selected anticancer proteins was performed using AutoDock Suite software. PyMOL and Discovery Studio Visualizer are used to determine the best matching conformations suggesting the compound's ability to inhibit these proteins and protect the body from cancer development.

Keywords: Solvent effect; Anti-cancer; DFT Topology; ADMET

Graphical abstract