I C R A A C S

INTERNATIONAL CONFERENCE ON RECENT ADVANCES IN APPLIED CHEMICAL SCIENCES

ICRAACS – 2019

EDITORS

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SREE SEVUGAN ANNAMALAI COLLEGE

(Accredited with 'B' Grade by NAAC)

(Affiliated to Alagappa University,Karaikudi)

Devakottai – 630 303.

DEPARTMENT OF CHEMISTRY

IN CELEBRATION OF THE GOLDEN JUBILEE

INTERNATIONAL CONFERENCE ON RECENT ADVANCES IN APPLIED CHEMICAL SCIENCES (ICRAACS – 2019)

6TH SEPTEMBER, 2019

Organized by

DEPARTMENT OF CHEMISTRY

SREE SEVUGAN ANNAMALAI COLLEGE
(Accredited with 'B' Grade by NAAC)
(Affiliated to Alagappa University, Karaikudi)
Devakottai – 630 303.

PREFACE

Of all charitable deeds, establishing educational institutions to cater to the educational needs of the people irrespective of their caste, creed and status is the best deed. In consonance with this dictum, Sri. O.RM.M.SP.SV.AN. Annamalai Chettiar, under the aegis of the Sri.SV.Annamalai Chettiar Educational Trust, established a prestigious college in Devakottai to provide quality education to the students in and around Devakottai. This noble gesture cried a halt to the exodus of students to far off places. That the College was called Sree Sevugan Annamalai College shows his profound filial piety. Affiliated to Madurai- Kamaraj University, this higher seat of learning came into existence in 1970.

Department of Chemistry was established in the year 1974, with a view of imparting scientific innovations and creativity among the students of the rural area. The Department has a well-equipped laboratory with sophisticated instruments. The Department has organized various students' enrichment programs like State level Quiz competition, Association meetings, Guest lectures, Industrial visits, etc. At present, the Department has highly qualified Faculties actively engaged in teaching as well as research in frontier areas of Chemistry and has published research papers in reputed National and International Journals. With rich experience of teaching and research, the Department focuses on enhancing Chemistry education with global perspective. The Department has an excellent academic record. The Alumni of the Department are eminent researchers at National and International Institutions, Reputed Pharmaceuticals and Chemical Industries.

Now, we feel proud in organizing for the first time an International Conference in Recent Advances in Applied Chemical Sciences on 6th September, 2019. The Conference

aims to provide vibrant opportunities for research/students to share their research experiences, research results, ideas, review of various aspects and practical development experiences. The Conference will mainly focus on the following topics which include invited, plenary and topical lectures of eminent researchers from various Institutions. Experts working in the areas like Polymeric and composite materials, Organic synthesis, Inorganic materials, Thin film/ Magnetic/Optical/ Semiconducting materials, Nano Materials, Smart Materials, Sensors, Environmental analysis and Miscellaneous topics are invited to participate and deliver lectures highlighting recent advances in their field of research. The response from the invited speakers, research scholars and other faculty members has been overwhelming.

We express our sincere thanks to the Management for their financial support to organize this Conference. We are thankful to our beloved Principal for her sustained support and guidance. We thank all the invited speakers, scientists, delegates from all parts of our country and all volunteers for their cooperation, help and moral support.

Organizing Committee

ICRAACS - 2019

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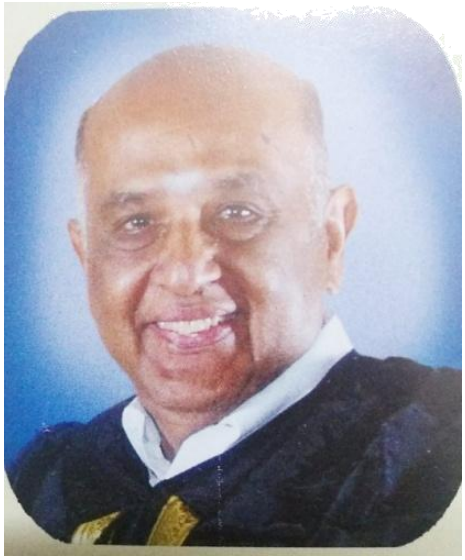


MESSAGE

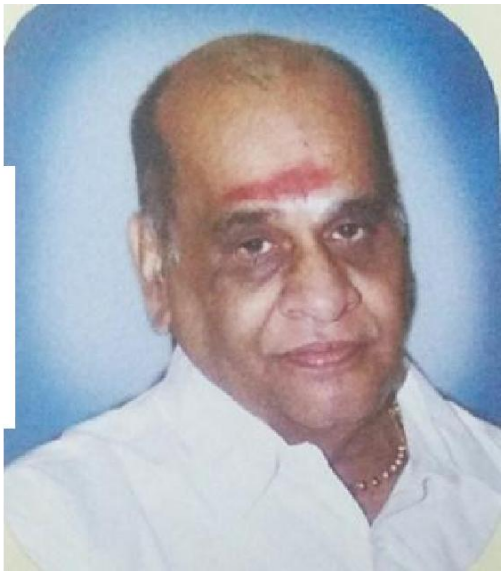
I feel great joy in wishing the **International Conference on Recent Advances in Applied Chemical Sciences (ICRAACS - 2019)** organized by the Department of Chemistry of our College a grand success.

I am sure it will serve as a platform for the Scientists, Research Scholars and Students of the Nation to share their research and practical experiences, and their knowledge in the field of Applied Chemical Sciences.

I congratulate the Organizers for their great efforts.

(AN. LAKSHMANAN CHETTIAR)

Sri. A. S. SEVUGAN CHETTIAR
Vice-President
Sree Sevugan Annamalai College



MESSAGE

It gives me immense pleasure to know that the Department of Chemistry of our College is organizing an **International Conference on Recent Advances in Applied Chemical Sciences (ICRAACS - 2019)** to bring together renowned Scientists and Research Scholars from different parts of the world to exchange their knowledge and application of Chemical Sciences with our students and others from the neighbourhood.

I wish the event a grand success and congratulate the Organizing Committee for the giant leap in the annals of the Department.

(A. S. SEVUGAN CHETTIAR)

Smt. A. S. SANTHI ACHI
Secretary
Sree Sevugan Annamalai College

MESSAGE

It is a pride moment for me to share my hearty wishes to the Department of Chemistry of our College for organizing the **International Conference on Recent Advances in Applied Chemical Sciences (ICRAACS - 2019)** in our premises.

The world is changing for betterment every day with numerous new inventions and innovations in all spheres of human life. More than the theoretical principles, the application oriented sciences contribute much to the sophisticated life of man.

I am sure that this Conference will showcase the best knowledge of the Scientists of the world to Research Scholars and Student fraternity. I congratulate the entire team for organizing such a conference in our College which will be fruitful to all the stakeholders.

My best wishes.

(A. S. SANTHI ACHI)

Dr. S.CHINTHAMANI VASTHI RANI
M.Sc., M.Phil., B.Ed., Ph.D,
Principal
Sree Sevugan Annamalai College

MESSAGE

I am extremely delighted to learn that the Department of Chemistry of our College is organizing an **"International Conference on Recent Advances in Applied Chemical Sciences" (ICRAACS – 2019)** on 6th of September 2019 on the occasion of the Golden Jubilee Celebration of Sree Sevugan Annamalai College.

The International conference aims to deliver a platform for the young researchers to develop and bring forth the latest advances in all areas of chemical science including the interfaces with related disciplines such as biology, medicine, and material science. In this regard, it is appropriate that the Department of Chemistry, has taken efforts to arrange this International Conference with invited lectures from eminent personalities in India and abroad with paper presentation by academicians, scientists, scholars, and industrialists.

I am sure that all the delegates would be greatly benefited by the deliberations of this conference with many innovative ideas.

I wish the Conference a grand success.

(Dr. S.CHINTHAMANI VASTHI RANI)

Dr. G. BHUVANALOGINI
Assistant Professor
Convener – ICRAACS - 2019

WELCOME TO THE DELEGATES

On behalf of the Staff and Students of the Department of Chemistry, Sree Sevugan Annamalai College, Devakottai, I am pleased to extend a hearty welcome to all the delegates of **the "International Conference on Recent Advances in Applied Chemical Sciences" (ICRAACS – 2019)** on 6th September 2019 which is organized to celebrate the Golden Jubilee Year of Sree Sevugan Annamalai College, Devakottai.

Though the conference announcement was at short notice, there was an overwhelming response. About 83 technical papers and 3 Invited Lectures were received during this short notice of time. These cover a wide range of topics and are programmed to be deliberated in 3 sessions.

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

I wish the delegates for enjoyable and memorable stay at Devakottai.

(Dr.G.BHUVANALOGINI)

INVITED LECTURES

Electrospun Nanomaterials for Dye Sensitized Solar Cells

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Abstract

Electrospun Nanomaterials have a high surface area with interconnected pores which enable to have significant attention in recent years and are considered as promising candidates to many hi-tech applications, particularly energy conversion and storage devices. These materials can be prepared by a simple and versatile electrospinning technique. By this technique, one dimensional nanostructured organic, inorganic and hybrid materials of controlled dimension can easily be produced. This presentation will focus on working principle of electrospinning and the influence of variable parameters such as electric potential, flow rate, polymer concentration, distance between the needle and target screen, temperature, humidity and motion of the target screen on the formation of electrospun materials. Further, special attention will be focused on the development of electrospun TiO_2 based photoanodes, CNFs based counter electrodes and ionic liquid incorporated electrospun polymer membrane-based electrolyte for dye-sensitized solar cells (DSSCs). These materials have very good photovoltaic performance than the same obtained by other conventional techniques.

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ROLE OF SUGAR INDUSTRIAL PRODUCTS FOR MAKING GREEN ATMOSPHERE

Dr. RAMESH DURAISAMY

Associate Professor, Department of Chemistry,
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Arba Minch (Ethiopia)

Abstract

Sugarcane (*Poaceae Saccharum*) is a tall tropical perennial grass that grows to between 2-6 m height. Sugarcane is used to produce a range of food products including sugar, molasses and golden syrup. More than 145 million tons of sugar (sucrose) is produced per year in about 120 countries; sugar production in Asia probably adds more than ten million tons to this total. Annual consumption is expanding each year by about two million tons. Around 60 - 70 % is produced from sugarcane with the remainder from sugar beet. The main product of sugarcane is raw sugar, made from the juice of the cane, and molasses which is a by-product of the sugarcane refining process. Biofuel ethanol can also be produced from sugarcane, which is an alcohol made by fermenting the sugar and starch components of plant materials using yeast. Ethanol can be used for food products but is also used as a biofuel. Bioethanol can be used in its pure form but is commonly added to gasoline to reduce vehicle emissions. The paper industry has a significant impact on the climate from deforestation to greenhouse gas emissions to the extensive use of water and energy. Timber harvesting for papermaking accounts for 37% of the destruction of forests, which are critical to storing carbon and cleaning the air. A tree-free paper made from sugarcane bagasse, which provides a carbon neutral paper option at an affordable price. Also, the bio-fertilizer is produced from the filter cake (by-product during the clarification of cane juice), which is the replacement of inorganic fertilizers. Thus, the sugar industrial products are considered as alternation biomass resource for the biofuel's, which an alternative eco-friendly fuel than petroleum conventional fuel.

Keywords: *Bagasse, Bio-fuel, Bio-fertilizers, Eco-friendly, Ethanol, Filter cake, Molasses,*

Nanomaterials for Biomedical Applications: *In silico* and *In vitro studies*

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Abstract

Nanotechnology plays a key role in the field of medicine. Metal nanoparticles showed good efficient in the field of pharmaceutical fields such as tissue engineering, biosensor, drug delivery etc. There are several methods such as chemical, son chemical, greener etc. have been used to synthesis the various metal nanoparticles which possessed unique physical/chemical properties and biological activities compared to bulk materials. The nanoparticles have been used for diverse biomedical applications including antibacterial, anticancer, anti-inflammatory and antiparasitic as well as drug delivery vehicle by using *In vitro* and *In vivo* analyses. However, they are not effective to cure the disease due to have some severe side effects to normal cells and low efficacy and poor drug delivery. To overcome these barriers, effective drug delivery system with safe, affordable and efficacies for diseases is highly imperative. In this talk, synthesis of metal nanoparticles by chemical method using reducing and stabilizing agents, greener method using plant extracts with their antibacterial and anticancer activities are discussed. Moreover self assembled nanoparticles synthesis with their drug delivery and computer simulation method will also be discussed.

Keywords: Metal nanoparticles, *In vitro, In Silico*, Drug delivery, Self assembled nanoparticles.

ABSTRACTS OF THE PAPERS PRESENTED IN THE CONFERENCE

Graphene oxide doped zinc oxide – a material for supercapacitor

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Abstract

Functionalization of graphene oxide can fundamentally change the priority of graphene oxides. The resulting chemically modified graphene could then potentially become much more adaptable for a lot of applications. There are many ways in which graphene oxide can be functionalized, depending on the desired application.

Zinc oxide (ZnO) is an important transition metal oxide with hexagonal crystal structure has attracted increasing attention owing to potential use as electrode materials. Nano crystalline ZnO is expected to possess many improved properties than those of micrometer-sized ZnO particles. A number of synthetic methods have been developed to prepare ZnO as well as ZnO-based composites with tunable surface morphologies and characteristic pseudo capacitance behaviour.

Herein we report grapheme oxide doped zinc oxide by microwave has drawn much attention to emphasize the structure activity relationship of ZnO material which accentuates the importance of surface properties on the charge storage performance. Further our studies show that, in addition to the parameters such as surface area and pore size, suitable surface morphology of ZnO is also an essential parameter for exhibiting higher pseudo capacitance.

Key words: Grpahene oxide, Zinc oxide, supercapacitors

Synthesis, characterisation and applications of thiourea doped KDP crystals

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Abstract:

Non linear optical (NLO) materials have acquired new significance with the advent of a large number of devices utilizing solid-state laser sources. Several NLO materials have been used for this kind of Technological applications. The Potassium di-hydrogen phosphate (KDP) one of NLO material having superior non linear optical properties has been exploited for variety of applications. In the present investigation we have grown KDP crystals from aqueous solution with thiourea, as an additive an organic non linear optical material. Single crystal of pure and thiourea doped KDP were grown from aqueous solution by slow evaporation method. The incorporation of thiourea in the grown crystals was qualitatively analyzed from FT-IR and UV-VIS studies .The presence of various functional groups and optical transparency were identified. The mechanical stability has been assessed to calculate the mechanical strength of the material in order to check its suitability for device applications.

Keywords: Crystal growth, NLO material, organic dopants, Refractive index, Microhardness

Introduction

Non –linear optic (NLO) materials plays a major role in photonics. Photonics involves the application of photons for information and image processing [1]. The important commercial NLO material Potassium di hydrogen phosphate (KH_2PO_4) was one among the earliest materials were exploited for their NLO properties. KDP finds widespread uses frequency doubles in laser applications, electro- optic switching and modulates organic crystals can have a very large nonlinear susceptibilities relative to inorganic crystals , but exhibit low damage threshold and poor process ability.[2, 3] Amino acids are interesting NLO materials for doping. They exhibit NLO property because they have a donor $NH2^+$ acceptor $COOH^-$ and the intermolecular charge transfer is also possible. Modifications in optical and physical properties of KDP by doping of amino acids such as L-arginine [4], L-lysine [5] L-alanine [6] and L-theonine [7] have been studied. The use of special additives is an effective way to accelerate the growth rate. Usually different organic inorganic compounds are used as additives in industrial crystallization and positive effect of some organic additives for the growth of large size crystals is widely known. [8]

The reason for choosing the organic additive of thiourea is due to the well known non-linear optical NLO and ferroelectric nature, respectively. The strength and deformation characteristics of the grown crystals were studied by hardness testing using diamond pyramid indenters [3] . Anbukumar et al. [4] had made attempts to study the micro hardness of pure KDP family crystals. In this present work, incorporation of thiourea in KDP crystals were grown from the aqueous solutions added with thiourea and the grown crystals were subjected to FT-IR, optical transmission and micro hardness studies

In this present work, incorporation of thiourea in KDP crystals were grownfrom the aqueous solutions added with thiourea and the grown crystals were subjected to FT-IR, optical transmission and microhardness studies. The reason for choosing the organic additive of thiourea is due to the well known non-linear optical NLO and ferroelectric nature, respectively [9,10]. The strength and deformation characteristics of the grown crystals were studied by hardness testing using diamond pyramid indenters [11] Anbukumar et al. [12] had made attempts to study the micro hardness of pure KDP family crystals.

2 Materials and Method

2.1 Experimental Procedure

To grow the single crystals of KDP, the procured salt of KDP from LOBA chemicals Pvt. Ltd was re crystallized several times for further purification and then used to grow the single crystals by the slow evaporation method.The starting materials namely KDP and thiourea were of AR grade and the growth process was carried out in aqueous solution. The calculated amount of salts of KDP and thiourea (3&5 mole %) was dissolved in Millipore water. This solution was then stirred well for more than six hours using a magnetic stirrer and filtered using Whatman filter paper. The prepared solution was kept in the dust free atmosphere. The optically good quality single crystal of Pure and thiourea doped KDP (KDTU) with different morphologies a and transparencies were harvested from the mother solution .The crystals of different sizes with similar morphologies due to doping are shown in Fig.1 (a)and 1(b). Optically good quality single crystal of dimension 5.3X2.7X 2.0 mm^3 were harvested after the period of 2-3 weeks.

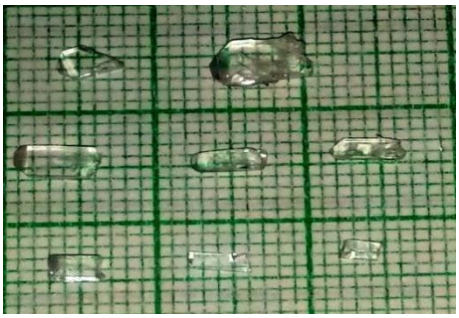


Fig .1 a) Photograph of 5 mol% thiourea doped KDP crystals

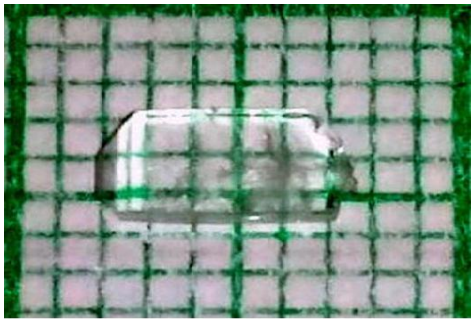


Fig .1b) Photograph of 3 mol% thiourea doped KDP crystal

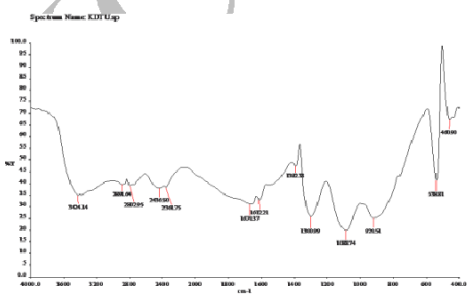
3 CHARACTERIZATION STUDIES

Incorporation of thiourea in KDP (KDTU) was subjected to different characterization studies such as FT-IR, UV-Vis spectral studies and mechanical stability of the sample was tested using micro hardness analysis.

3.1 Fourier Transmission Infrared (FT-IR) analysis

The FT-IR analysis is a technique that provides information about the chemical bonding or molecular structure of materials.The FT-IR spectrum of KDTU crystals is shown in the Fig 2(a)&2(b).The absorption peaks correspond to the molecular group vibrations. The FT-IR spectrum of incorporation of thiourea in KDP was recorded using Perkin Elmer in the region 400cm-1 to 4000cm-1.

The different bonding such as o-p-o bending and K-o stretching vibration, p=o-H stretching vibration, O-H and O-H stretching present in pure KDP are in continuum with KDTU crystals with small shift in frequency. In KDTU crystal a broad envelope positioned in between 2800 to cm-1 corresponds to symmetric and asymmetric mode of NH_2 grouping, this may be due to thiourea.[13] The FT-IR frequency assignment s of pure and KDTU crystals is listed table 1.



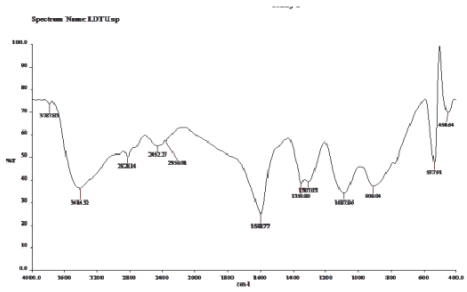


Fig .2a FT-IR spectra of 5 mole thiourea doped KDP crystal

Fig .2b FT-IR spectra of 3 mole thiourea doped KDP crystal

Pure KDP(cm-1)	Thiou$_{3\%}$KDP(cm-1)	Thiou$_{5\%}$KDP(cm-1)	Assignments
2500-3800	2452	2436	O-H stretching
1696	1598	1612	O-P-OH stretching
1302	1307	1300	P=O stretching
1098	1087	1088	P-stretching
909.4	909	920	P-O-H stretching
300-650	537	538	O-P-O bending
320-450	454	460	K-O stretching

Table 1 FTIR –Frequency Assignment of Pure and thiourea doped KDP crystal

3.2 UV-visible spectral studies

UV-visible spectral studies of grown KDTU crystal were carried out using shimadzu 1601 UV-V spectrophotometer. The UV-visible absorbance spectrum of 5 mole% KDTU crystal was recorded in the wavelength region from 200 to 1100 nm[14] .The absorption spectrum reveals that in thiourea added crystal there is strong absorption in 200 to 300nm which was in good agreement in previous result. The relationship between refractive index of KDTU crystal and photon energy in eV is shown in the Fig. 3(a) & 3(b). Using the formula Eg=hc/λ , where h is planck's constant and the c is velocity of the light . It was seen than that band gap energy is 3.16eV for pure KDP and 3.5 eV for doped KDP. Therefore the improved band gap energy of 3.5 eV and better crystal transparency in doped KDP can attributed to the presence of thiourea [15] .The optical parameters are listed in table 2.

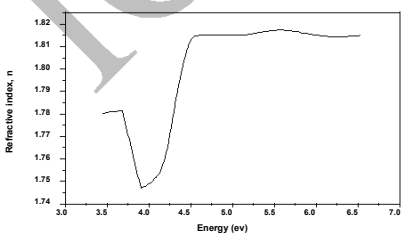


Fig 3a Plot of versus photon energy (ev) for title crystal

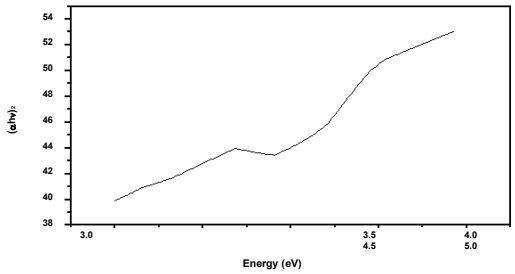


Fig .3b Plot of refractive index versus photon energy (ev) for title crystal

Parameters	KDP+Thiourea(5 %)	Potassium Dihydrogen [19]Phosphate[KDP]
Refractive index	1.79	2.04
Extinction Coefficient	4.77x10^ -5	34.09
Ac susceptibility	0.25	9.6×10^{-5}
Eg e^{nx}	3.5 Ev	3.16
Dielectric constant	3.22	36.14

Table 2.The values of Optical parameters

3.3 MICROHARDNESS

The micro-indentation test is a useful method for studying the nature of plastic flow and its influence on the deformation of the material. Also the hardness of the crystal is depending on the type of chemical bonding, which may differ along the crystallographic direction. [**16**]. The indentations were made on the plane of Pure and doped KDTU crystals at room temperature with the load ranging from 25, 50 and 100g using a Vickers hardness tester fitted with a Vickers diamond pyramidal indenter and attached to an incident light microscope. The indentation time was kept as 10 s for all the loads. For each load, several indentations were made and the average value of the diagonal length was used to calculate the micro hardness.

The Vickers hardness number H**v** was calculated using the equation [17,18] given as follows:

$$Hv = 1.8544 \times P/d^2 \ kg/mm^2 \quad \text{---------- (1)}$$

Where P is the applied load in kilogram and d is the diagonal length of the indentation impression in mm and 1.8544 is a constant ofa geometrical factor for the diamond pyramid.

Fig. 4b shows that the hardness of the grown pure and doped KDTU single crystal increases with increase of load. Using Meyer's law we calculate the Meyer's index (n) to analyze the nature of the material. The size of indentation and load are related through Meyer's law [16].

$$P = k_1 d^n \quad \text{---------- (2)}$$

From the slope of log P vs. log d and P Vs d^2 plots are shown in Fig. 4a,4c. From the plots it gives the estimated n value. Since the value of n is larger than 1.6, it's belongs to the soft material category, the hardness of the material is found to increase with the increase of load. Also the elastic stiffness constant is calculated using Wooster's empirical formula [18], which is given by

$$C_{11} = (Hv)^{7/4} \quad \text{---------- (3)}$$

This gives an idea about the tightness of bonding between the neighboring atoms. Since the value of n is larger than 1.6, its belongs to the soft material category, the hardness of the material is found to increase with the increase of load. The calculated values of W and H_0 and $C_{11}$are given in Table 3. The results indicate that the mechanical properties of KDP crystal could be increased with optimum selection of the organic additive.[19]

Fig .3b Plot of refractive index versus photon energy (ev) for title crystal

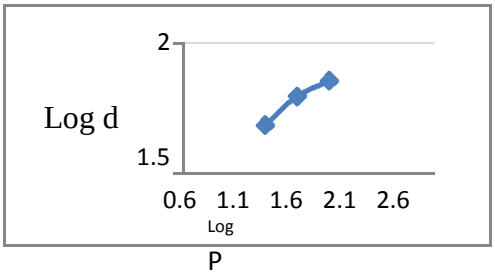


Fig .4a Plot of log P versus log d for title crystal

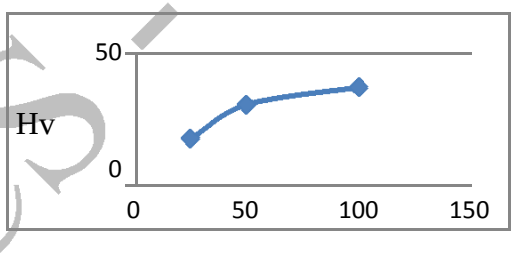


Fig .4b Plot of P Vs Hv for title crystal

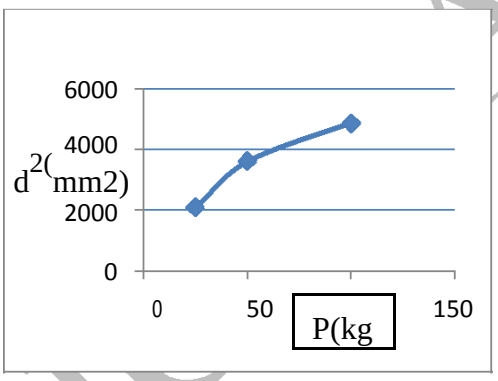


Fig .4c Plot of P Vs d^2 for title crystal

s.no	Load (Kg)	Hv (Kg/m m^2)	Ho	$C_{11}x10^{14}$ Pa
1.	25	0.022	15.55	121.7666
2	50	0.025534	29.2	366.7921
3	100	0.038002	36.25	535.5364

Table 3.The values of Mechanical parameters for different loads

4 Conclusion

KDP crystals with organic additives were grown from aqueous solutions by slow evaporation method. FTIR analysis confirmed the incorporation of different functional

groups of thiourea as dopant. It has also been observed that the cut off wavelength is almost the same for pure and additive added KDP crystals .The band gap of grown crystal was found to be 3.5eV demanded for optical applications.[20] . In the case of KDP, the hardness is found to increase with the incorporation of thiourea and it also found to suppress the inclusions and improve the quality of crystal with higher transparency to the solution.

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Hirshfeld surface analysis of some arylhydrazones

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ABSTRACT

Single crystal X-ray structures of some intra-molecularly hydrogen bonded arylhydrazones were reported from our laboratory. The type of hydrogen bonding in these systems are known as Resonance Assisted Hydrogen Bonding (RAHB). The unusual stability of the hydrogen bonding is due to the planarity of the pseudo six membered ring formation. Hirshfeld surface analysis of for these systems are carried out. The intermolecular interactions which stabilize the crystal structures are discussed in detail and the relative contributions of each interactions are quantified. Differences in the packing interactions among the crystal structures are discussed.

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Aloe vera assisted facile green synthesis of Reduced Graphene oxide

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Abstract

An eco-friendly and effective reducing agent viz., Aloevera is used to convert Graphene Oxide (GO) to reduced Graphene Oxide (RGO). The oxygen scavenging property of Aloevera (AV) extract is successfully utilized to remove oxygen functionalities on GO. The synthesis RGO was optimised by varying the concentrations of AV. The synthesised RGO samples were characterised using UV–Vis , FT-IR and its XRD studies. 12.5g of AV demonstrated a maximum reduction efficiency as evidenced by the disappearance of the band at 300nm in the UV–Vis spectral studies. The significant decrease in intensity of peaks due to alkoxy and hydroxyl groups at 3456 cm^{-1} of GO in RGO sample as per FTIR studies also confirmed the above conclusion. This conclusion was further substantiated by the disappearance of (001) peak in XRD studies. Thus our method provides a simple, efficient, eco friendly method for reduction of GO.

Keywords: *GO, RGO, Aloevera, UV-Vis, FTIR and XRD*

A Comparison of Results From Theoretical And Experimental Studies of N´-(3-Phenylallylidene) Isonicotinohydrazide And N´-(3-(4-Methoxyphenyl) Phenylallylidene) Isonicotinohydrazide

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N´-(3-phenylallylidene) isonicotinohydrazide (**1**) and N´-(3-(4-methoxyphenyl) allylidene benzohydrazide(**2**) were synthesised and characterised by ^{1}H and ^{13}C NMR spectra. Theoretical calculations were performed for some possible conformations. From the optimised structures, HOMO, LUMO energy gap geometrical parameters were derived. The vibrational frequencies in the ground state have been calculated using DFT methods and compared with the observed frequencies. Non linear optical (NLO) behaviour of the hydrazides was investigated by the determination of the electric dipole moment μ, the polarizability α, and the hyperpolarizability β using B3LYP method. The chemical shifts computed by ^{13}C and ^{1}H NMR analysis also show good agreement with experimental observations.NBO and AIM analysis were also made theoretically. The hydrazides were evaluated for their anti-microbial activities against 10 micro organisms. The hdrazides exhibited more activity against *staphylococcus aureus.* The antimicrobial screening results and evaluation of anticancer activity indicated that OCH_3 substituted hydrazide was the active one.

Key words: isonicotinohydrazide, HOMO, LUMO, characterisation, DFT method, antimicrobial activity

Bio synthesis of palladium nanoparticles using natural resource of *Ocimum Basilicum* leaf extract

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Abstract

Eco- friendly manner for synthesis of palladium nanoparticles were successively synthesized by aqueous extract of naturally occur *Ocimum basilicum*. Bio method aimed at manufacturing nanoscale materials as deals greatly development of additional methods as it is single step and reproducibility materials. The aqueous extract of *ocimum basilicum* has a reducing capability of nanoparticle production. In bio-compatible way, *ocimum basilicum* extract reduce palladium ion solution into form palladium nanoparticles. As prepared palladium nanoparticles remained monitored by various analytical techniques such as UV-Visible spectroscopy, Fourier Transform infrared spectroscopy, Scanning electron microscopy with Energy dispersive X-ray spectroscopy, X-ray diffraction and Transmission electron microscopy.

Keywords: *$PdCl_2$, Ocimum basilicum, Palladium nanoparticles, Bioreduction, UV- Visible, FTIR, XRD, SEM with EDAX, TEM.*

Synthesis of ZnO Nanoparticles using Termite and Ant Mount Extract: *In vitro* Evaluation of Antioxidant and Photovoltaic Efficacy

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ABSTRACT

ZnO nanoparticles (ZnO NPs) have received tremendous attraction in various fields such as cosmetics, food packaging, photovoltaic, thermoelectric, constructions and therapeutic agents due to its cost effectiveness and biocompatibility. ZnO NPs have been synthesized from biological sources (extracts from termite and ant clays). Generally termites and ants construct the mounts for their habitats using their bodies, salivary glands and soil. Termite and ant mounts consist of some bioactive elements present in the soil or salivary glands of termite and ant. So far the termite and ant mount extracts has been used for the synthesis of ZnO nanomaterials. The prepared ZnO nanoparticles were characterized using spectroscopic and microscopic techniques. Results of antioxidant and photovoltaic potential showed that ZnO NPs synthesized through biogenic route exhibited optimum free radical scavenging activity, reducing power and solar cell J-V Characteristics with response to antioxidant and photovoltaic potentials respectively. Over all results of this present study conclude that ZnO NPs produced through biogenic source showed potent antioxidant and solar cell efficiency when compared to chemical synthesis, which might be due to the biologically active organic compounds adhered to the surface of the synthesized nanoparticles

Key words: *Zinc oxide nanoparticles; Termite soil; Ant soil; Antimicrobial activity; Antioxidant and Photovoltaic activity.*

Acknowledgement: RUSA 2.0

Anisomeles malabarica: Novel adsorbent for the removal of heavy metal ion from simulated wastewater

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Due to industrialization and urbanization, excessive release of heavy metals into the atmosphere has posed a major issue globally. Heavy metal ions do not degrade into harmless end products unlike organic pollutants. Heavy metal pollution exists in aqueous wastes of several industries. Treatment procedures for removing heavy metals from wastewater include precipitation, membrane filtration, ion exchange, adsorption, and co-precipitation/adsorption. Studies on the effluent treatment bearing heavy metals disclosed that adsorption was an extremely efficient method for removing heavy metals from wastewater and activated carbon was commonly used as an adsorbent. The need for secure and economical methods to remove heavy metals from contaminated waters in recent years has required low-cost agricultural waste by-products. An adsorbent prepared from *Anisomeles malabarica* leaves which was activated with sulphuric acid that was assessed for its efficacy in removing Fe (II) ions from simulated wastewater. The process parameters studied are agitation time, initial ion concentration, adsorbent dose, pH and temperature. The equilibrium data were correlated with Langmuir, Freundlich and Temkin, isotherm models. The adsorption followed pseudo-second-order rate equation and the rate is primarily regulated by intraparticle diffusion.

Dye removal from aqueous solution using sulphuric acid activated carbon developed from *Anisomeles malabarica* leaves

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In the textile, paper, rubber, plastics, leather and cosmetics, pharmaceutical, and food industries, more than ten thousand dyes have been commonly used. The discharge of colored wastes into the receiving water bodies not only impacts their aesthetic character but also interferes with sunlight transmission and thus decreases the photosynthetic activity. As dyes are designed to resist breakdown with time, exposure to sunlight, water, soap, and oxidizing agent cannot be easily removed by conventional treatment techniques due to their complex structure and synthetic origins. Adsorption is one of the physical-chemical methods, which is found to be the most simple and economical to remove the dyes from effluents. In the present study, activated carbon prepared from *Anisomeles malabarica* leaves have been used as an adsorbent for potent dye removal. The effects of operating parameters such as initial dye concentration, adsorbent dosage, pH, agitation speed, contact time, particle size, and temperature were studied.

Corrosion Inhibition Efficiencies of Poly Aminothiophenols on Mild Steel in HCl

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Abstract

The applicability of conducting polymer to enhance the corrosion resistance on metals in an acid environment is gaining greater significance as corrosion inhibitors. In the present work, the isomers of poly(aminothiophenol) are synthesized by *in situ* chemical oxidative polymerization method and the synthesized polymers are characterized using FT-IR, UV-VIS, XRD and SEM. The inhibition performance of the isomers of poly(aminothiophenol) on mild steel in 1M hydrochloric acid solution is studied by electrochemical methods and weight loss method and their results are compared. The results show that the inhibition efficiency is found to increase with increasing concentration of the inhibitor. The maximum inhibition efficiency is observed for all the three polymers at the optimum concentration of 500 ppm. The inhibition action of poly(aminothiphenol) is explained in terms of adsorption which can form protective films on the surface of the mild steel. The results obtained from the electrochemical methods are in good agreement with the weight loss method. The result clearly show that the isomers of poly(aminothiophenol) act as a good corrosion inhibitor on mild steel in 1M HCl solution.

Keywords: *Aminothiophenol, Conducting polymers, Corrosion, Mild steel, Electrochemical studies.*

Bio template chitosan assisted Ni doped ZnO/reduced graphene oxide nanocomposite modified GCE for sensing of heavy metal ions

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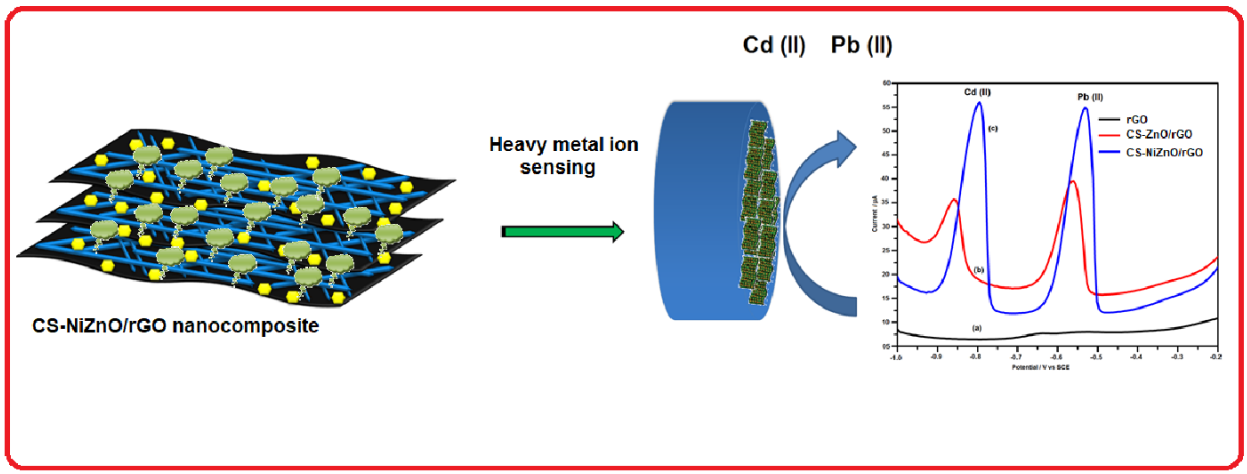
ABSTRACT

Bio template chitosan assisted Ni doped ZnO/reduced graphene oxide (CS-NiZnO/rGO) nanocomposite modified glassy carbon electrode (GCE) has been used for simultaneous determination of heavy metal ions such as lead and cadmium ion. Functional group idendification, surface morphology and crystalline properties of the CS-NiZnO/rGO were characterized by FTIR, SEM and XRD respectively. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) had been used to investigate the electrochemical behavior of CS-NiZnO/rGO nanocomposite toward lead (Pb) and cadmium (Cd) ion. DPV measurements showed a linear relationship between oxidation peak current and concentration of Pb and Cd in phosphate buffer (pH 7) over the concentration range of 10 nM to 100 nM. With Comparing to bare GCE and CS-ZnO/rGO, the CS-NiZnO/rGO nanocomposite showed higher catalytic activity toward electrochemical oxidation of Pb and Cd ion.

Key words: RGO, ZnO, lead, cadmium, SEM, DPV.



GREEN SYNTHESIS, CHARACTERIZATION AND ANTIBACTERIAL ACTIVITIES OF ZINC OXIDE NANOPARTICLES FROM THE LEAF EXTRACT OF *SOLANUM MELONGENA*

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Abstract

Zinc oxide nanoparticles have been successfully synthesized using a simple and efficient method. Furthermore, we have demonstrated that the use of a natural, low cost biological reducing agent, Leaf extract of Solanum melongena can produce Zinc oxide nanoparticles in aqueous solution at room temperature. The characterization of zinc oxide nanoparticles revealed surface morphology, size and shape of nanoparticles depends on the extract concentration. Based on the kinetic studies, together with evidence obtained from UV-Visible, FTIR, XRD and SEM it is assumed that the phytochemicals which are present in Solanum melongena leaf extract is responsible for the formation of Zinc hydroxide which produces Zinc oxide on annealing at 400°C for 3 h in Muffle furnace. Bacterial toxicity assessment revealed that biogenic zinc oxide nanoparticles synthesized using *Solanum melongena* leaf extract possessed antibacterial activity against the microbial strains Klebsiella pneumoniae *and* Staphylococcus aureus. The process for the synthesis of zinc oxide nanoparticles in large scale using *Solanum melongena* leaf extract may have commercial viability and to develop studies in the surface between biology and material science.

Key words: *ZnO nanoparticles, Solanum melongena, Antibacterial activity, Klebsiella pneumoniae and Staphylococcus aureus*

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SYNTHESIS AND CHARACTERIZATION OF POLY (3,4-ETHYLENE DIOXYTHIOPHENE)–ZINC OXIDE NANOCOMPOSITES FOR PHOTOVOLTAIC DEVICES

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Abstract:

Due to the demand for sources of inexpensive renewable energy, solid polymer solar cells have attracted a large amount of research. The proposed research described the fabrication of Poly (3,4-ethylenedioxythiophene)-Zinc oxide nanocomposites photovoltaic devices. Poly (3,4-ethylenedioxythiophene)-Zinc oxide nanocomposites prepared by chemical oxidative polymerization method, in which the weight of ZnO was varied from 0.5 to 2.5g. The structure and morphology of the composites were characterized by Fourier Transform Infrared (FTIR) spectroscopy, Ultraviolet-Visible (UV-Vis) absorption spectroscopy, Field Emission Scanning Electron Microscopy (FESEM) and electrochemical studies. The FTIR and UV-Vis results show that the composites were strong interaction between PEDOT and ZnO nanoparticles. The FESEM results suggested that the composites were a transparent and rippled silk wave appearance. The EDAX analysis showed the different ratio of carbon, oxygen, sulphur and zinc. I-V characterization indicates that the incorporation of ZnO nanoparticles in composites exhibits enhanced the power conversion efficiency of the composites from 0.16 to 0.4%. Our recommended cost effective and efficient polymer metal oxide photovoltaic devices stand out as sustainable future generation solar cells.

Keywords: *Nanocomposites, UV, FTIR, AFM, FESEM, Electrochemical studies, Solar cell.*

SYNTHESIS AND CHARACTERIZATION OF COBALT(II) COORDINATION POLYMERS CONSTRUCTED BY AMINO ACID

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Coordination polymers, cyanometallates and clathrates have significance as an important class of solid-state materials. Many researchers were attracted by the variety of structures, properties, composition, synthesis and easy modification of the coordination polymers. MOFs have exceptional porosity and a wide range of potential uses including gas storage, separations, and catalysis. We report here the preparation of cobalt MOFs containing amino acid and diacid derivatives of the type M-L-gly, M-L-phe and M-L-asn (M-Co and L-phthalic acid, Amino acid – Gly, Phe, Asn). To prepare MOFs with different amino acids, a previously reported method (Ross J. Marshall et al., 2016) was modified by using amino acids containing Co(II).

The prepared MOFs were confirmed by IR spectra. The stretching frequency of C= O group from amino acids were appeared in the range of 1600-1660 cm^{-1}. The stretching frequency of C=O group present in phthalic acid were confirmed by a peak raised in the range of 1700-1750 cm^{-1}. The Cobalt – Oxygen linkage were confirmed by the appearance of a peak present in the range of 540-560 cm^{-1}. The bands in the range 400-460 cm^{-1} confirmed the formation of Co - N linkage in the Co-L-Gly, Co-L-Phe and Co-L-Asn whereas 480-500 cm^{-1} in the range were assigned to Co - Cl linkage in the Co-L-Gly, Co-L-Phe and Co-L-Asn. The TG curve indicates that all the prepared MOFs were thermally stable up to 200 ^{o}C. The initial weight loses in Co-L-gly at temperatures below 100°C are due to the evaporation of surface-adsorbed DMF and moisture. A decompositions curve at 247 ^{o}C indicates the removal of ligand. The MOF Co-L-gly exhibits a rapid weight loss above 300 ^{o}C indicating the fast decomposition of the MOF structure. In Co-L-gly, gradual weight loss occurred from 250 ^{o}C to 300 ^{o}C followed by a sharp weight drop above 300 ^{o}C, suggesting a two-step decomposition. The MOF Co-L-Phe was thermally stable up to temperature of 200 ^{o}C. The gradual weight loss occurred from 200 ^{o}C to 400 ^{o}C. The decomposition at 280 ^{o}C may be due to phthalic acid.

The cobalt MOFs showed good antimicrobial activity against various pathogens. Gram- positive and Gram-negative bacterial activities were studied and their zone of inhibition were recorded. The increased lipophilic character of these MOFs seems to be the reason for their enhanced potent antibacterial activity. There are other factors such as solubility, conductivity, and bond length between the metal and the ligand which may contribute to their activity. Co - MOF containing amino acids (glycine and phenylalanine) and dicarboxylic acid (Phthalic acid) showed better activity at all almost all the levels of concentration (60 and 90µL). Cobalt- MOFs showed a very good zone of inhibition against all the microbes. Among the tested microbes E.coli showed good zone of inhibition towards all the MOFs. When compared to the control (Nil) all the tested microbes and the prepared MOFs were showed good activity. The zone of inhibition was depending upon the concentration and ligands.

PHOTOINDUCED ACTIVATION OF $Co^{III}(tn)_2Cl(L)^{2+}$ ON AQUEOUS TiO_2 SUSPENSIONS UNDER VISIBLE-LIGHT ILLUMINATION IN BINARY SOLVENT MIXTURES

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Abstract

Interfacial electron transfer at nanomaterial (nm) TiO_2/ $Co^{III}(tn)_2Cl(L)^{2+}$ interface by employing binary solvent mixtures has been probed by designed solution and chemical reactions in H_2O/methanol (or isopropanol). The distinct photoreduction of Co^{III} at λ = 254 nm excitation leads to possible reduction route on the surface due to solvent influence is presented for cobalt(III) complexes $Co^{III}(tn)_2Cl(L)^{2+}$ (where L = *p*-*F*, *H*, *p*-OEt, and *p*-OMe) by nm-TiO_2 particles; $Co^{III} + TiO_2 + h\nu \rightarrow TiO_2\ (h,e^-) + Co^{III} \rightarrow TiO_2\ (h) + Co^{II}$. In this the strategy of adsorption/accumulation of $Co^{III}(tn)_2Cl(L)^{2+}$ at the active surface is achievable by the addition of organic cosolvent and the interfacial charge transfer is competent at nm-TiO_2/Co^{III} were generated by photoreduction probed by HRTEM-SAED, SEM-EDAX and X-ray mapping analyses. Accompanying the adsorption and subsequent photoreduction the deposition/dissolution balance of $Co^{III}(tn)_2Cl(L)^{2+}$ ion and Co^{II}_{aq} provided the possibility of cyclic progression in solvent adapted medium. An obscurity on binary solvent improved $\Phi_{Co(II)}$ in terms of correlation analyses using solvent empirical parameters ε_r, Y, E_T^N, DN^N, α, β and π^* provides a model to appreciate solvent medium participation. Surface morphologies prove the operative foraging by nm-TiO_2 particles in the photoreduction of $Co^{III} \rightarrow Co^{II}$ in binary solvent medium.

Keywords: *Photoreduction, solvent effect, regression analysis, quantum yield*

DEVELOPMENT OF ELECTRODE MATERIALS FOR ASYMMETRIC SUPERCAPACITOR APPLICATIONS

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Abstract

The energy issue is the most important topic of the twenty first century. An excessive reliance on the combustion of non-renewable fossil fuels brings not only ecological problems but also harsh ongoing impacts on the global economy and society[1]. There is a pressing requirement for cost-effective, efficient, and environmentally benign energy conversion and storage (ECS) devices that can power energy demanding areas, ranging from portable electronics (e.g., cell phones, camcorders, laptops) to transportation (e.g., electric vehicles, hybrid electric vehicles) and even stationary. Typical ECS devices include fuel cells, solar cells, photoelectrochemical water splitting cells, batteries (especially Li-ion batteries) and supercapacitors[2-8]. The performance of these energy devices relies strongly on the properties of their nanostructured materials. New development in the field of nanomaterial chemistry is believed to hold the key to further breakthroughs in ECS systems.

Interest in supercapacitors as a main or a sub-power source for various applications requiring high power density such as electric vehicles, UPS systems and windmills has increased. The use of supercapacitors in the applications described above is thus far insufficient because the energy density is only one tenth of that in a secondary battery. Therefore, many researchers have investigated methods to improve the working voltage, specific capacitance, and energy density of supercapacitors. High surface area conducting nanofibers make electrospun materials attractive as electrodes for batteries or in electrochemical supercapacitor applications. The traditional method for preparing $LiCoO_2$ can result in inhomogeneity and irregular grain growth, whereas, the sol–gel method provides pure material with good crystallizability, homogeneity and uniform size [9]. Electrospinning techniques have been very successful for making inorganic nanofibers utilizing the sol–gel method. Lithium-ions (Li+) are transported between electrodes through the electrolytic medium during charge and discharge. Compared to conventional film based morphology, nanotubes and nanofibers are expected to have improved electrode properties due to their high surface areas and 1D nanostructure properties, and therefore should provide higher rates of electron transfer [10]. In addition, their entangled network allows easy access of the ions to the electrode/ electrolyte interface. The electrospun nanofibers of $LiCoO_2$ demonstrated

improved electrode properties as the result of high surface area[11, 12]. Hence there is a need to have cheaper electrode materials for asymmetric supercapacitor applications.

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NANOSILICA REINFORCED IMINE SKELETAL PHENYLENE BASED POLYBENZOXAZINE ($nSiO_2$/PBZ) NANO COMPOSITES

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Abstract:

A series of nanosilica reinforced polybenzoxazine ($nSiO_2$/PBZ) were developed from various phenyl pendant pyridine core imines via Mannich condensation. The structure of the products obtained was analyzed via FTIR and their optical behavior analyzed by UV-Visible spectroscopic techniques. The curing behaviour measurements by DSC, showed single glass transition temperature (Tg) for PBZ and the nanocomposites have high glass transition temperature than the neat PBZ. The fire retardancy was also increased with increase the concentration of nanosilica content as confirmed by TGA. The UV-Vis absorption bands at the region of 310–370 nm and from Photoluminescence analysis, the fluorescent emissions were observed in the wavelength range of 330–550 nm. The successful developments of nanocomposites were conformed from the characteristic peaks corresponding to $nSiO_2$. The reports from thermal and optical properties show that the $nSiO_2$/ PBZ nanocomposites can be employed in the field of advanced composite materials.

Keywords: *Benzoxazine, $nSiO_2$, imine, curing, nanocomposites and thermal stability.*

Ecofriendly Coatings using Aryl Pendant Pyrene core Imine Skeletal Nanosilica reinforced Polybenzoxazine (*n*SiO_2/PBZ) Nanocomposites

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Abstract

A new series of aryl pendant pyrene core imine skeletal nanosilica reinforced polybenzoxazine (*n*SiO_2/PBZ) nanocomposites were developed using benzoxazine monomer (BZs) and *n*SiO_2 through the *in-situ* sol-gel process. The resulting nanocomposites were confirmed by FT-IR. Their optical behaviors and fluorescent studies done by UV-Visible spectroscopic techniques and Photoluminescence spectrophotometer. From the glass-transition temperature (T_g) and curing behaviors from TGA and DSC, shown good thermal stability and high char yield. The low water absorption and good thermal stability, showed the ecofriendly usage of these hybrids in large applications in industrial areas. The developed nanocomposite was then characterized by the UV-Vis spectroscopy, photo luminescence (PL), impedance analyzer, XRD and SEM techniques. These developed hybrids may be expected to find a wide range of application in the fields of aerospace, microelectronics and environmental applications.

Keywords: *Ecofriendly coatings, benzoxazine, imine, nanosilica, nanocomposites and low water absorption.*

Environment pollution and public health:

ANION-RESPONSIVE POLYMER GELS FOR THE DETECTION AND REMOVAL OF FLUORIDE ION

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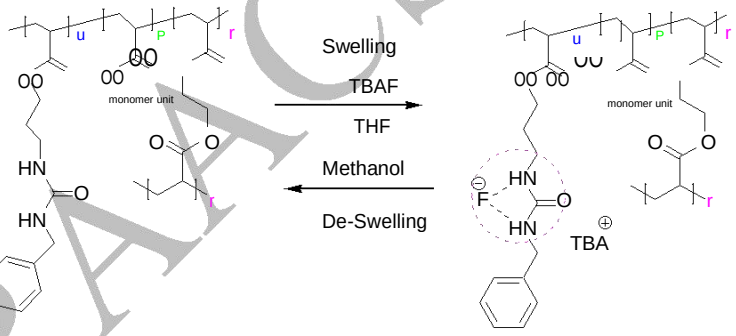
Abstract

Stimuli-responsive polymer gels that can change their volumes drastically in response to various external physical and chemical stimuli have been of much interest due to various applications for actuators, drug delivery and micro fluidic devices. Among them, the stimuli-responsive polymer gels to specific chemical substances have been much studied due to application of molecular recognitions for material sciences. Thus, the guest molecules as the external stimuli have been still limited owing to difficulty in designing host–guest systems with high affinity in water. This prompted us to design novel anion-responsive polymer gels performed in non-polar media by incorporation of anion receptors into the lipophilic polymer chain. Complexation of specific anions with the receptors should enforce free counter cations to entrap in the inside of the polymer gels, which induces osmotic pressure and electrostatic repulsion to expand the gel. Non-polar media should allow us to use hydrogen bonds between the anion receptors and the target anions, which might increase binding affinity compared to that in water. Thus, anion-responsive polymer gels were prepared by incorporation of urea into poly (octadecyl acrylate) gels, and the colours and volumes were changed selectively in the presence of fluoride by complexation in THF as given in fig 1. Hence, they should be highly useful in an anion detecting and removing technology in prevention of pollution.



Dry Gel Swelled Gel Fig. 1

***Keywords**: Anion-responsive polymer gels, anion detecting and removing technology.*

Reference: 1.Krishnamurthi, J.; Ono, T.; Amemori, S.; Komatsu, H.; Shinkai, S.; Sada, K. *Chem. Commun*. **2011**, 1571-1573.

Thiophenyl Pendent Cardanol End Capped Imine Skeletal Nanosilica Reinforced Polybenzoxazine (*n*SiO_2/PBZ) Nanocomposites

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Abstract:

A novel Thiophenyl pendent cardinal end capped imine skeletal nanosilica/polybenzoxazine (*n*SiO_2/PBZ) nanocomposites were designed and developed via thermal polymerization. The benzoxazine monomer was obtained from Thiophenyl pendant aromatic dimine blended with formaldehyde and cardanol which then undergoes polymerization to form polybenzoxazine nanocomposites and reinforced with varying percentages of *n*SiO_2.The synthesized PBZ nanocomposites were characterized by FT-IR. The PBZ nanocomposites have shown high thermal stability, glass transition temperature (T_g)

and low dielectric constant. The values of dielectric constant of the nanocomposites were decreased with increased silica content. The reduction in percentage water uptake may be associated with the inherent hydrophobic nature of Si–O–Si network present in the *n*SiO_2/PBZ hybrid systems. The optical properties ascertained from the UV-Vis absorption bands at the region of 300–350 nm and strong emissions were observed in the wavelength range of 300–550 nm from Photoluminescence analysis. The homogeneous morphology of the nanocomposites caused from the good interfacial interaction between the embedded *n*SiO_2 particles and PBZ nanocomposites as evidenced by SEM and AFM images. The molecular level dispersion of *n*SiO_2 particles in the polybenzoxazine matrices was evidenced from morphological studies.

Keywords *Cardinal, benzoxazine, nanosilica, thermal polymerization, polybenzoxazine, nanocomposites and thermal stability.*

APPLICATION AND CHARATERIZATION OF FIBER REINFORCED EPOXY POLYMER COMPOSITES

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Abstract

Organic Cotton Fibers (OCF) was prepared from the Organic Cotton Fiber by chemical and physical method. The Organic Cotton Fibers were characterized by the Fourier Transformed Infra Red spectroscopy (FTIR), Field Emission scanning electron Spectroscopy (FE-SEM) and High Resolution-Transmission Electron Microscope (HR-TEM). Epoxy polymer based composites reinforced with OCF at different loading and wt. % were prepared by compression moulding. These OCF-composite samples were characterized by mechanical characterization, thermal analysis, moisture uptake behavior and scanning electron microscopy (SEM).

Keywords: Fibers; Mechanical properties; Chemical analysis; Compression moulding

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Custom-made Sulfonated poly(vinylidene fluoride-co-hexafluoropropylene) Nanocomposite Proton Exchange Membranes for Vanadium Redox Flow Battery Applications

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Abstract

Polydopamine functionalized exfoliated molybdenum disulfide (PD-MoS_2) embedded sulfonated poly(vinylidene fluoride-co-hexafluoropropylene) (SPVDF-co-HFP) nanocomposite proton exchange membranes (PEMs) are fabricated by solution casting method for vanadium redox flow battery (VRFB) applications. The prepared PD-MoS_2 nanosheets are probed in terms of FT-IR, XRD and FT-Raman whereas SPVDF-co-HFP/PD-MoS_2 nanocomposite PEMs are characterized by surface morphology (FE-SEM and AFM), thermal and mechanical stability, proton conductivity and vanadium ion permeability. FE-SEM images of SPVDF-co-HFP/PD-MoS_2 membranes showed a dense and homogeneous structure. The nanocomposite PEMs exhibited adequate ion exchange capacity and water uptake. Further, the interfacial-formed acid-base pairs between PD-MoS_2 and SPVDF-co-HFP matrix effectively reduces the swelling ratio and vanadium ion permeability, however increasing the proton conductivity of the PEMs. The dispersing ability of PD-MoS_2 content in the SPVDF-co-HFP matrix is improved the surface roughness, thermal and mechanical stability of the composite membranes. Particularly, the SPVDF-co-HFP/PD-MoS_2-1membrane exhibits highest proton conductivity of 6.10×10^{-3} Scm^{-1} at 80 ºC and lowest vanadium ion permeability of 1.05×10^{-8} cm^2s^{-1}.Overall results suggest that the SPVDF-co-HFP/PD-MoS_2-1 composite PEMs found to be suitable alternative for commercially costly Nafion in VRFB applications.

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Synthesis and Characterization and Antimicrobial Screening Studies of Mixed Ligand Schiff base Complexes

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Abstract

Schiff bases are one of the well-known chelating ligands. They are able to easily coordinate to various metal ions. They are versatile compounds synthesized from the condensation of a primary amino compound with aldehydes or ketones and have a wide variety of applications in many fields including analytical, biological, medicinal, organic, inorganic chemistry and as catalysts in several reactions. At present, the concept of mixed ligand complexes is emerging in the fields of bio-inorganic and coordination chemistry particularly in the fields of pharmaceutical and medicinal fields. The synthesis of new antimicrobial agents is an emergency medical issue using the mixed ligand complexes. Moreover, the study of coordination chemistry of transition metal ions with particularly copper(II), cobalt (II), nickel(II) and zinc(II) complexes is drawing the attention among the bio-inorganic chemists. Hence, in this work, a seines of Cu(II) , Co(II), Ni(II) and Zn(II) mixed ligand complexes have been synthesised by incorporating the bio-ligand isoniazid and characterized them by Elemental, UV-Vis., IR, NMR , Mass and molar conductance methods. The main aim of the production and synthesis of any antimicrobial compound is to inhibit the causal microbe without any side effects on the patients. In that aspect, it has been tried to screen the synthesised complexes against a few bacterial and fungal strains. It is found that these complexes are having higher activity than the free ligands.

Keywords: *Schiff bases, Transition metal, Antimicrobial screening and Molar conductance.*

Synthesis, Spectral Characterization and Molecular Docking Studies of New Imine Base Binuclear Metal Complexes

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Abstract

A Novel and simple approach to the synthesis of tetradentate Schiff base ligand formed by the condensation of 9,10-phenathrenequinone with 4-phenylthiosemicarbazide by reflux method. Schiff base complex show eminent catalytic activity in abundant reactions in presence of moisture. The transition metal [Cu (II), Ni (II) and Ru (III)] complexes was synthesized by treating absolute alcoholic solution of the ligand with appropriate amount of metal salts (2:1) (M:L) ratio. The complexes were distinguished by elemental analysis, Infrared, Spectrofluorimter, NMR and Electronic spectral data. The free ligand and their metal complexes were screened for their antimicrobial activities against the following species: *Klebsiella pneumoniae*, *Escherichia coli*and *Staphylococcus aureus*. A comparative study of minimum inhibitory concentration (MIC) values of the Schiff base and its complexes indicate that the metal complexes exhibit higher antibacterial activity than the free ligand. Moreover, the molecular docking analysis has been performed to calculate the binding energy and to understand the nature of binding of complexes with BSA protein (PDB ID: 4f5s). Among these complexes Copper (II) complex shows higher negative value which indicates that the binding energy of this Cu (II) complex with 4f5s is greater.

***Keywords**: Schiff base, 9,10-phenathrenequinone, 4-phenylthiosemicarbazide and Molecular docking.*

Hydrothermal Synthesis of CuO-SnO_2 Nanoparticles and Its Application for the Photodegradation of Rhodamine B

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Abstract

In this work, CuO-SnO_2 nanoparticles (CuO-SnO_2NPs) were developed through a facile hydrothermal technique followed by calcination process at two different temperatures *viz.* 800°C and 700°C respectively. The phase structure, surface morphology and optical properties of the as-prepared CuO-SnO_2 NPs were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier Transform Infrared (FTIR) and DRS-Ultraviolet spectroscopy. The photocatalytic activity of the as-prepared CuO-SnO_2 NPs was assessed by the photodegradation RhB dye under UV-light irradiation. The results demonstrate that CuO-SnO_2NPs displayed excellent photocatalytic performance for the reduction degradation of RhB aqueous solution. The effects of various factors such as variation of pH, catalyst concentration and initial substrate concentration as well as reaction kinetics were investigated. The results showed that 95% degradation of RhB (5 mg/L) can be achieved with 0.05 g/L ZnO-SnO_2 NPs in 30 min under UV-light irradiation. The work is expected to shed new light on the development of novel nanostructures for gathering visible light energy and on the improvement of new photocatalytic materials for the exclusion of environmental pollutants.

Keywords: Hydrothermal, CuO-SnO_2, Nanoparticles, Organic Pollutants.

Synthesis, Spectroscopic Investigation and Biological Studies of Metal (II) Chelates of Novel Schiff Base

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Abstract

In this work, Cu(II), Ni(II), Mn(II) & Zn(II) complexes of 3,3'-(1E)-5,8-dioxa-2,11-diazadodeca-1,11-diene-1,12-diyl) diphenol derived from 2-[2-(2-aminoethoxy) ethoxy] ethanamine and 3-formylphenol have been synthesized. The Metal-Ligand molar ratio is 1:2. The synthesized compounds were characterized by elemental analysis, molar conductance, magnetic susceptibility measurements, IR, UV- Vis., ^{1}H- NMR and EPR spectral data. The FTIR spectra showed that the ligand behaves as a dibasic tetradentate by coordinating through one azomethine nitrogen, one phenolic oxygen atom in N_2O_2 fashion. Magnetic measurements and electronic spectral data of the chelates suggest that all the complexes are square planar geometry. The mono electrolytic nature of the chelates was confirmed by molar conductance data. The ligand and their metal complexes were screened the antioxidant activities of the complexes were also investigated through their scavenging effect on DPPH radicals. The obtained IC50 value of the DPPH activity for the copper complex was higher than the values obtained for the other complexes. In addition, the mode of DNA binding of the ligand and complexes was analyzed theoretically using cyclic voltammetric measurement. These investigations, when explored in details on our synthesized complexes, strongly evidence intercalation as the binding mode. These efficient complexes may be further developed into DNA probes.

Keywords: *Schiff base, Transition metal complexes, Antioxidant, DNA Binding*

Synthesis and characterization of metal complexes having E-N-(4-bromobenzylidene)-5-methylbenzo[d]thiazol-2-amine

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Abstract

Synthesis of modified and new desired compounds has an everlasting demand. The present work emphasizes on the one pot three compounds synthesis of E-N-(4-bromobenzylidene)-5-methylbenzo[d]thiazol-2-amine obtained by the reaction of 2-amino-6-methylbenzotiazole derivatives with 4-bromobernzaldehyde and methanol in the presence of triethylamine. All the newly complexes *viz*., Cu(II), Zn(II), Ni(II), Co(II) were synthesised and isolated as solid products and characterized by elemental analysis as well as spectral techniques like IR, UV-Vis. ^{1}H NMR, ^{13}C NMR, EPR, ESI-Mass and magnetic susceptibility measurements. The DNA (CT-DNA) binding study of the synthesized metal complexes was carried out by UV-Vis. absorption and viscosity methods. Oxidative DNA cleavage activities of the complexes were studied with supercoiled (SC) pUC19 DNA using gel electrophoresis. The antimicrobial activity of the synthesized Schiff base complexes was done by disk diffusion method. In view of the biological activity of the Schiff base and its metal complexes it has been observed that the antimicrobial activity of the Schiff base was increased on complexation with metal ion. Molecular docking studies were also performed to explore the binding modes and orientations of the complexes in the DNA helix.

Keywords: *Schiff base, Gel electrophoresis, Molecular docking and Transition metal*

STUDIES ON THE ELECTRODEPOSITION OF SILVER FROM PHOTOWASH WASTE

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Abstract

The recovery of silver from photowash waste is a method of industrial waste treatment which is to be considered not only from the environmental point of view, but also for the protection of the valuable resources. The present study deals with the electrodeposition of silver besides the use of the reducing agents like hydrazine dihydrochloride, sodium selenite, sodium hypophosphite and sodium -metabisulphite in small measures. Thiourea, phenyl thiourea and p-tolyl thiourea have been tried as brighteners. A Hull cell study was used to optimize the recovery of silver from the photowash waste. The effective electrolysis is reported for best reducer and brightener concentration with graphite and stainless steel as anode and cathode respectively. The recovered silvers purity is estimated through volumetric procedure and is found to be in the range of 98.5 to 99%.

Preparation and Characterization of Copper Oxide NPs using Datura Stramonium Plant Extract by Chemical Route

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Abstract:

CuO nano particles were synthesized by simple co-precipitation method by using Datura Stramonium leaf extract. XRD studies show that the prepared sample has polycrystalline in nature with monoclinic structure having preferential orientation along (0 0 2) plane. It is observed from the SEM images and XRD patterns that the grain sizes of the structures were nearly 50 nm. The optical transmittance in the visible range is greater than 55%. The optical band gap of the synthesized CuO nano particles is 1.140 eV is decreased compared to bulk CuO band gap energy 1.21 eV. FTIR analysis shows that the prepared films have functional groups. We believe that our proposed co-precipitation method nano structured CuO Nps are promising for gas sensor and opto electronics applications.

Keywords: *CuO, plant extract, Co-precipitation, XRD, SEM, FTIR, UV and Semiconductors.*

SYNTHESIS OF BIOACTIVE NANOPARTICLE AND ITS APPLICATION FOR IMPROVED ANTIBACTERIAL ACTIVITY

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ABSTRACT:

At present, more synthetic antibacterial nanoparticles are developed and applied on textiles because of their novel properties and low material consumption of nanoparticles. To replace the synthetic chemicals from antibacterial finishing, research is ongoing to find bioactive agents from natural products. Recent research shows that seaweed can be used for isolation of antibacterial agents. Along with antibacterial activity, seaweed also is used for nutritional purposes and to remove metal ions from wastewater. In the present investigation, an attempt was made to extract bioactive substance using acetone as a solvent and characterized by Fourier transform infrared (FTIR) spectroscopy. Furthermore, the extracted bioactive substance was subjected to Atomic absorption spectroscopy (AAS) for heavy metal removal and applied on cotton fabric for antibacterial property.

KEYWORDS: Seaweed, Antibacterial activity, FTIR, AAS.

An Effect of 'Mn' Addition on ZnO Thin Films by Successive Ionic Layer Adsorption and Reaction (SILAR) Method

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Abstract:

Mn doped Zinc Oxide (ZnO) thin films have been successfully coated onto glass substrates at various Mg doping level such as 0%, 5%, 10% and 15% by Low cost SILAR coating technique. The film thickness was estimated using weight gain method and it revealed that the film thickness increased with Mn doping concentration values. The prepared film structural, morphological and optical properties were studied using X-ray diffraction (XRD), scanning electron microscope (SEM) and UV-Vis-NIR spectrophotometer respectively. The structure of the films were found to be hexagonal structure with polycrystalline in nature with preferential orientation along (002) plane. X-ray line profile analysis was used to evaluate the micro structural parameters such as crystallite size, micro strain, dislocation density and stacking fault probability. The calculated crystallite size values lies between 41 nm – 36 mn. The crystallite size values are decreased with increase of Mn doping concentration values and maximum value of crystallite size was estimated at 41 nm at doping concentration of 0%. Morphological results showed that the concentration of the Mn has a marked effect on morphology of the ZnO thin films. The optical studies revealed that the band gap can be tailored between 3.63 eV to 3.72 eV by altering doping concentration. EDAX studies showed that the presence of Zn, O and Mn content.

Keywords: *Zinc Oxide, Thin Films, Structural Studies, Morphological Studies, Optical Properties.*

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Structural, Optical and Magnetic Analysis on Co-precipitated Spinel Ferrites (MFe_2O_4) (M=Ni, Co, Zn, Cu)

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Abstract

Nanostructured spinel ferrites (MFe_2O_4) (M = Ni, Co, Zn, Cu) were successfully synthesized by co - precipitation method and annealed at 700°C for 4 hours. The structural, optical and magnetic properties of the synthesized samples were characterized by XRD, FT-IR, UV-DRS and VSM analysis. X-ray diffraction study (XRD) confirms that the formation of single phase spinel structure with the space group Fd-3m. The crystalline size for the synthesized nickel ferrite, cobalt ferrite, zinc ferrite and copper ferrite is found to be 27nm, 31nm, 25nm, 30nm respectively. The Fourier transform infra-red (FT-IR) spectroscopy shows the transmission bands which are assigned to the vibration of tetrahedral and octahedral complexes. The UV– DRS study confirms that the samples are active in the visible region and the band gap values of the nickel ferrite, cobalt ferrite, zinc ferrite and copper ferrite are 1.85eV, 1.4eV, 2.1eV, 1.56eV respectively. The vibrating sample magnetometer (VSM) is used to obtain the hysteresis parameters.

OPTICAL PROPERTIES OF Co DOPED ZnO THIN FILMS

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ABSTRACT

Pure and Co doped ZnO thin films were prepared by Chemical Bath Deposition (CBD) method with the doping concentration of 0.01 M and 0.1 M of Co. The optical properties of the as deposited films have been characterised using UV-Visible spectroscopy and Photoluminescence spectra. UV-Vis absorption and transmittance spectra showed that all the films are highly transparent in the visible region and in the case of doped ZnO thin films, d-d transition was observed in the violet region due to the existence of crystalline defects and grain boundaries. The energy band gap were found to decreases as the Co concentration increases with the range of 3.8-3.67eV. The photoluminescence (PL) spectra of all the samples exhibited a broad emission in the visible range.

Solvent Effect, Spectral and DFT Studies of Some 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 novel 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 **1** to **4** 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: *Absorption, Fluorescence, nano SiO_2, DFT, chemical shift.*

Spectral and Antimicrobial studies of someBis-dimedone derivatives

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ABSTRACT

Medicinal chemistry is the application of chemical research techniques to the synthesis of pharmaceuticals. Medicinal chemistry explains the design and production of compounds that can be used for the prevention, treatment or cure of human and animal diseases. Bisdimedone derivatives, acridines, acridinediones, xanthene derivatives show antimicrobial activities against certain bacterial and fungal strains. Xanthylium and the carbonyl compound xanthone are derived from xanthene. Xanthenes are important because of their use in medicine and they possess biological activities.

Antibiotic chemistry has recently undergo explosive growth due to the advancement of various isolation methods like HPLC, TLC, CCD, ion-exchange and structural determination like NMR, mass, X-ray crystallographic methods. The use of specialized microseparation methods and various instrumental techniques coupled with electron impact, chemical ionisation and mass spectroscopy led to the rapid identification of numerous complicated molecular structures.

Keywords: *NMR, X-ray, Antibacterial, Antifungal.*

DFT and Physico-chemical studies of some imidazole derivatives

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Abstract

The photophysical properties of imidazole derivatives namely 2-(2, 4-difluorophenyl)-4,5-dimethyl-1-p-tolyl-1H-imidazole and N, N-dimethyl-4-(4,5-dimethyl-2-phenyl-1H-imidazol-1-yl)benzenamine, synthesized from an unusual four components assembling, were studied in several solvents. From the spectral results, it was found that there is equilibrium between neutral species and monocationic (MC) species in polar aprotic and polar protic solvents. The basicity of the solvent, C_β or C_{SB} has a negative value, suggesting that the absorption and fluorescence bands shift to lower energies with increasing electron-donating ability of the solvent. Therefore, resonance structures 1b & 2b has the positive charge located at the nitrogen atom stabilized in basic solvents. Imidazole derivatives have attracted considerable attention because of their unique optical properties. These compounds play very important role in chemistry as mediators for synthetic reactions, primarily for preparing functionalized materials. Imidazole nucleus forms well-known components of human organisms and used as laser, polymer stabilizer.

Keywords: *Absorption, Fluorescence, DFT, chemical shift.*

Fabrication of Antibacterial cotton using microcapsules of Thymol

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Abstract:

Natural fibre cotton is more prone to microbial attack due its hydrophilicity there by, microbial infestation produces unpleasant odour,stains and deterioration to fibre. Antimicrobial finish is an essential criterion for cotton to protect the weaver from microbes and also necessary for medical, surgical and healthcare products. Antimicrobial finish can be done by different technologies of which microencapsulation is a novel techniques where the antimicrobial agent known as core material was encapsulated by wall material. The advantages of this method are cost effective and durable to washing process.In this study the antimicrobial finish was done on cotton using Thymol as core material and gum acacia a biodegradable polymer as wall material. Microcapsules of thymol prepared by co-acervation technique was studied by light microscopic analysis & FT-IR analysis. The microcapsules were impregnated on fabric by pad-dry cure method.The Scanning electron microscopic analysis proved the existence of microcapsules on fabric. The antibacterial studies was done for gram negative bacteria E.Coli by agar diffusion method. Thymol an antibacterial agent is capable to destroy the E.Coli by penetration into cell wall.

Keywords : Antimicrobial,Co-acervation, Microencapsulation, E.Coli,Thymol.

"INCLUSION COMPLEXES AS FOOD PACKAGING APPLICATION"

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Abstract

Microbial contamination causes the deterioration of food materials during storage and transportation. Antimicrobial packaging, a form of active packaging was extended the shelf life of food product in a mild preservation way while maintaining its nutritional and sensory qualities. With the concerns for the environment and food safety, Glutinous Rice starch (GRS) with biodegradable polymers (PVA and PLA) and Essential oils (EOs) a plant-derived antimicrobial substance are used as food-contact material. The encapsulation techniques were used for prevention of volatility and increase the stability of essential oils by inclusion mechanism with cyclodextrins. GRS/PVA/PLA based electrospun nanofibrous cyclodextrin inclusion complexes were applied as active food packaging application. Antimicrobial activity of nanofibrous films were carried out.

Keywords: *Essential oils, Antimicrobial packaging, biodegradable polymers, encapsulation, inclusion complexes*

CHARACTERISATION AND CORROSION STUDIES OF Ni-W ALLOYS

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Abstract:

Nickel tungsten alloys has a large pool of applications in industry field. Corrosion of those alloys stands an issue for long term uses. This work attempts to prepare a nickel tungsten more corrosion resistant alloy by electro deposition. Rather than adding additive or coating a inhibitor this method is more tranquil work just by changing the parameters. Nickel tungsten alloy was prepared by electro deposition bath, the bath was optimized by varying the temperature, current and pH for best results in corrosion protection. Characterization of so done variations were reported by XRD, SEM, Hull Cell. The corrosion studies was done by potentio- dynamic studies and nyquist plots. The variation done in bath, their characterization differences and their corrosion resistant qualities were tabled and showed in graph. The best corrosion resistant variant and its preparation parameters was reported.

***Key words**: XRD, SEM, Hull Cell, Electro deposition*

EFFECT OF AZEOTROPIC SOLVENT MIXTURE PRETREATMENT ON THE COMPOSITE FABRIC

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Polyester Fabric has lot of Commercial importance in the Textile Industry. Blending synthetic Fibres with natural fibres can offer Fascinating properties to the blend with excellent dimensional stability, wear resistance and durable pleat retention. This paper will describe an investigation made on the process of pretreatment of polyester / Cotton Fabric to modify its physicochemical and dyeing behavior. Modification of the Fabric was carried out by treating the fabric with different time intervals and the treated fabric were subjected to various analytical investigations such as the surface modification. Using SEM, FTIR, X-Ray Diffraction method and thermal behavior by DSC.

Key words : Azeotropic solvent mixture, SEM, DSC, FTIR, XRD, Dyeability.

Fabrication of novel Cobalt selenide nanostructures for efficient photocatalytic degradation of antibotic drug

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Abstract

Novel Cobalt selenide nanoparticles (CoSe NPs) through a simple hydrothermal technique. The crystalline structure, morphology and elemental compositions were investigated by X-ray diffraction (XRD), Scanning electron microscopy (SEM), and Energy Dispersive X-ray spectroscopy (EDX) analysis. The photocatalytic activity of CoSe NPs was scrutinized for the degradation of Cefioxime (CF) under visible light irradiation. The obtained UV-vis spectroscopy results illustrate that CoSe NPs could degrade above 98% CF aqueous solution within 70 min of visible light irradiation. Radical trapping experiments revealed that the hydroxyl radicals (•OH) plays predominant for the degradation system. This study showed that engineering the interfacial structures could provide a scientific basis for the design of efficient photocatalysts.

Keywords: *Antibiotic drug, Photocatalyst, Nanostructure,Visible light.*

Design of Dye sensitized Graphene Oxide Nanoparticles – An Excellent Photocatalysis for degradation of Organophosphate Pesticides.

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Abstract

The photo-degradation of organic pollutants using solar light is an attractive chemical process for water pollution control. In this study, we synthesized a novel highly efficient Dye sensitized Graphene oxide (Dye GO) photocatalyst for degradation of organophosphate pesticides Methyl parathion (MP). The phase structure, surface morphology and optical properties of the as-prepared Dye GO was characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Raman, Fourier Transform Infrared (FTIR) and Ultraviolet spectroscopy. The photocatalytic activity of the as-prepared Dye GO was assessed by degradation of MP under visible light irradiation. The results demonstrate that Dye GO displayed excellent photocatalytic performance for the degradation of MP. The effect of various factors such as catalyst concentration and initial substrate concentration as well as reaction kinetics were investigated. Furthermore, it could be easily recovered by simple filtration process after the photo degradation process. The work is expected to shed new light on the development of novel nanostructures for gathering visible light energy and on the improvement of new photocatalytic materials for the exclusion of environmental pollutants.

Keywords: *Photocatalysis, Dye sensitization, Visible light, Pesticide.*

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Copper substituted stable layered electrode material for cost Effective sodium ion rechargeable battery

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Abstract

The development in the field of science and technology naturally tempt man in using and applying these developments to their daily life, creates a high demand for energy consumption. Sodium batteries are the types of secondary cells that use sodium-ion as charge carriers. The operation principle of a Na-ion battery cell is similar to its Li-ion analogue. In this work we have prepared The P2-type copper-substituted $Na_{0.66}Ni_{0.23}Cu_{0.1}Mn_{0.67}$ material was synthesized by simple solid state method. The X-ray diffraction analysis shows the successful accommodation of Cu into the host P2-struture. The microstructures of the as-synthesized $Na_{0.66}Ni_{0.23}Cu_{0.1}Mn_{0.67}$ were characterized by scanning electron microscopy (SEM) and HR-TEM, electrochemical properties are carried out with initial discharge capacity of 140 $mAhg^{-1}$ between 2.0V to 4.0 V at 0.1 C rate.

Investigation of corrosion resistance properties of Carbon steel in an aqueous environment by Iso leucine-Ni^{2+} system

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ABSTRACT:

The inhibition efficiency of Isoleucine-Ni^{2+} system in controlling corrosion of carbon steel in an aqueous environment has been investigated by weight-loss method. The formulation consisting of 300 ppm of Isoleucine and 30 ppm of Ni^{2+} offers 86 % IE. Statistical study of Synergism parameter showed that synergistic effect exist between Isoleucine - Ni^{2+} system. Potentiodynamic polarization study reveals that the Isoleucine - Ni^{2+}system function as mixed type inhibitor, predominantly cathodic in nature. The formation of protective film over the metal surface were investigated by AC impedance analysis.

Keywords: *IsoLeucine, Synergism parameter, Potentiodynamic polarization study AC impedance spectra.*

Improved cycle stability of $FePO_4$ coated $LiMn_2O_4$ cathode materials for rechargeable lithium ion batteries

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In this work, we have attempted to synthesize $FePO_4$ coated $LiMn_2O_4$ particles by sol–gel method. The structure and electrochemical performance of the surface modified $LiMn_2O_4$ cathode materials were characterized by using XRD, SEM, TEM, XPS, Cyclic voltammetry and Charge-discharge techniques. XRD studies revealed that coated $LiMn_2O_4$ did not show any change in the 2θ value of the peaks, lattice parameters and no impurities were detected. TEM and XPS results of $FePO_4$ coated over the surface of the core $LiMn_2O_4$ powder materials. The initial discharge capacity for $LiMn_2O_4$ was 125 mAh/g and declines to 70 mAh/g after 100^{th} cycle with a capacity loss of 44%. The fast capacity fading was ascribed to the contribution of Mn^{3+} ions for Jahn-Teller distortion during the cycling process. The charge/discharge capacities of surface modified $LiMn_2O_4$ cathode material have little reduced with increasing coating content. This result suggests that even for the $FePO_4$-coated spinel phase, only the Mn^{3+} contributes the charge/discharge capacities during the electrochemical reaction. The 2.0 Wt.% of $FePO_4$-coated $LiMn_2O_4$ exhibits initial discharge capacity of 106 mAh/g, but after 100 cycles only 17% capacity loss was obtained and the discharge capacity still maintains at 88 mAh/g. This cycling behaviour of the $FePO_4$-coated $LiMn_2O_4$ electrodes indicate the impact of $FePO_4$ coating significantly which improved the electrochemical performances. From these results, it is believed that the improved electrochemical performances of $FePO_4$-coated $LiMn_2O_4$ is attributed to the ability of $FePO_4$ layer in preventing direct contact of the active material with the electrolyte resulting in a decrease of electrolyte decomposition reactions and dissolution of active materials.

KEYWORDS : Cathode material, XRD, XPS, Charge/Discharge

FIRST PRINCIPAL CALCULATIONS OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF TRANSITION METALS DOPED MgH_2

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ABSTRACT

A group of Mg-based hydrides stand as promising candidate for competitive hydrogen storage with reversible hydrogen capacity up to 7.6 wt% for on-board applications. Efforts have been devoted to these materials to decrease their desorption temperature, enhance the kinetics and cycle life. Several attempts have been made to amend these materials to improve their properties, including doping them with other chemical components.

In the present study, relativistic spin polarized electronic band structure calculations are performed and the stability, the energy band structure, density of states, bulk modulus of the transition metals (Sc, Ti ,V and Ni) doped MgH_2 systems are calculated based on the first principles approach under the frame work of the density functional theory using the generalized gradient approximation (GGA-PBE). The formation enthalpy of MgH_2 is -0.58eV and the value is in good agreement with the previously reported theoretical work. It has been found that the formation enthalpy values for all the doped systems is negatively small compared to that of pure MgH_2 indicating that the destabilization happens in all the doped systems. Ni doped MgH_2 system has a lower formation enthalpy of - 0.44eV than other systems and therefore destabilization occurs more easily leading to a larger decrease in the desorption temperature .All the transition metal doped systems has higher bulk modulus in the range of (52-54)GPa compared with that of pure MgH_2 with B_0 value of 51.87GPa implying that the resistance to uniform compression increases for all the doped systems. The bonding between the dopant-hydrogen in all the doped systems is mainly covalent and the bond length of Ni doped MgH_2 is longer (1.912 and 2.017Å) compared to other systems and hence Ni doped MgH_2 has weaker bonding between Mg and H requiring less energy for the bond dissociation lowering the desorption temperature leading to reduced dehydrogenation energy. Thus Ni doped MgH_2 shows good performance for better hydrogen storage with a high volumetric and gravimetric storage capacity and can be used in fuel cells, batteries thermal energies and other environmentally friendly energy utilization applications.

ENHANCEMENT OF SILVER DOPED ZINC OXIDE NANOPOWDER BY HANDLING THE PRINCIPLE OF GREEN CHEMISTRY

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Abstract

The green synthesis of Ag capped ZnO nano particles were using tridax Procumbers leaf extract has become low-cost and eco-friendly method. The XRD pattern of Ag capped ZnO nano particles were analysed. The typical ZnO hexagonal wurtzite structure conforms according to the JCPDS card no.36-1451. The preferential orientation is along the (101) plane observed in the present work and also that the pre-dominancy of the (101) peak is not affected by the Ag doping. UV- visible spectrophotometer we found that the band was observed around 370- 380 nm which was identified as "surface Plasmon resonance band" and this band is ascribed to excitation of valence electrons of ZnO arranged in the nanoparticles. SEM of the Ag/ZnO sample shows that agglomeration has been taken place. FTIR identified the possible biomolecules responsible for the reduction of ZnO and capping agent of bioreduced ZnO NPs through particular bond vibrations peaks coming at defined wave numbers. The antibacterial studies indicated that the nanopowder have the ability to destroy gram-positive bacteria and gram-negative bacteria. The bactericidal effects of nano composites are explained by the formation of highly reactive oxygen species (ROS) (OH^-, H_2O_2 and $O2^{2-}$) on the surface of the nanomaterial which causes fatal damage to the bacteria. Thus, it is concluded that Tridax Procumbers leaf leaves could be successfully used for the biosynthesis Ag/ZnO NPs which are multifunctional.

Keywords: *Tridax Procumbers leaf, Green synthesis, biosynthesis Ag/ZnO NPs Antibacterial studies.*

ENHANCEMENT OF PHOTOCATALYTIC ACTIVITIES OF ZnO:Ag NANO POWDERS THROUGH THE ADDITION OF BAMBOO CHARCOAL

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The simple, low cost, easiness of synthesis and higher photodegradation activity of the ZnO:Ag/BC is used for wastewater treatment. ZnO:Ag/BC nanocomposite showed rapid and higher degradation of MB and MG as compared to dye removal of ZnO:Ag. The degradation rate constant of MB dye for ZnO:Ag is 0.0484 min^{-1} . It increases 1.28 times (0.0620 min^{-1}) for ZnO:Ag/BC nanopowders. Similarly in the case of MG dye the rate constant increases 1.34 times due to efficient natural adsorbent bamboo charcoal. The ZnO:Ag/BC nanocomposite proved as a promising photocatalyst towards harmful organic dyes and antibacterial agent against microorganisms.

Study on Physico-Chemical properties of Citrus (Lemon) and Citron (Narthangai)

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Abstract:

Citrus fruits are prized for their high content of vitamin-C and antioxidants. Citric acid is the predominant acid in Citrus fruits. Food and drug manufactures often use it as a preservative because it helps in maintain the stability of active ingredients. Excess citric acid is excreted in urine so it doesn't build up in your body.

Lemons are a healthy addition to freshly squeezed juices and homemade meals. In a 2017 clinical trial that appeared in the journal scientific reports, researches assessed the effects of fruit and vegetable juice on body weight with lemon juice as their primary ingredient.

The aim of current study was to screen and compare the physcio-chemical properties of lemon and citron. Fruits were collected washed, crushed and filter fresh juice was prepared and physcio-chemical properties were evaluated.

The pH of juice found in the range of 1.6 (lemon) and 2.0 (citron). The reducing sugar analysis showed that the higher content reducing sugar in citron than lemon. The total titrable acidity shows that lemon contains higher amount of citric acid than citron.

Key words: *lemon, citron, pH, Titrable acidity.*

SYNTHESIS AND CHARACTERIZATION OF *CALOTROPIS GIGANTEA* LEAF EXTRACT CAPPED ZnO BASED NANOPARTICLES FOR ENVIRONMENTAL FORTIFICATION

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ABSTRACT

The concept of green chemistry and engineering has provided a new platform for the environmentally propitious synthesis, non-hazardous to the environment and human health. Now-a-days synthesis of nano-materials with plant extracts have been a source of brainwave in designing commercial products for promising applications like biosensors, photo catalysis, antimicrobial and antioxidant technologies, etc. In the present study, we reported for the synthesis of *Calotropis gigantea* (*C. gigantea*) leaf extract capped ZnO based nanoparticles (NPs) by a simple soft chemical route via green approach. The resultant products were thoroughly analyzed using different analytical techniques such as UV-Vis NIR spectrophotometer, photoluminescence spectrometer, Fourier Transform Infrared spectrophotometer and X-ray diffraction technique. The observed properties were compared with uncapped ZnO based NPs counterparts and reported. The XRD patterns reveal that the synthesized NPs exhibit clear crystallization with (101) as a growth direction. The optical studies indicate that the *C. gigantea* capped ZnO NPs show higher band gap when compared to the uncapped NPs. In PL spectra, both uncapped and *C. gigantea* leaf extract capped ZnO NPs showed two peaks at 395 nm and 426 nm corresponding to band edge and interstitial impurities emission, respectively. The synthesized NPs are evaluated using its antimicrobial efficacy for two different human pathogenic organisms such as *Escherichia Coli* and *Staphylococcus aureus*. It is shown that the *C. gigantea* leaf extract capped ZnO based NPs exhibit better antibacterial activity against human pathogens when compared to uncapped one.

Alignment of Bent-Core Liquid Crystal Using Flexible Polymer Substrate

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A transparent flexible polymer film is chemically functionalized with a bent-core liquid crystal (BCLC) compound for effective alignment of the bulk BCLC sample at the substrate-LC interface. The surface attachment was achieved *via* a simple procedure which involved pre-treatment of the polymer film (commercial name: over-head projector film) using piranha solution followed by chemically attaching the BCLC compound through silane condensation reaction. Surface characterisation of the unmodified and BC modified flexible films was carried out through X-ray photoelectron spectroscopy (XPS), attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, contact angle (CA) and atomic force microscopy (AFM) techniques. The BC modified flexible substrates are analysed for their efficiency to orient the bulk LC sample. Remarkably, the chemically modified polymer substrates are highly efficient in vertically aligning both the BC and rod-like LC samples at the substrate-LC interface, in comparison to their unmodified and octadecyltrimethoxysilane modified counterparts. The described method is simple, reproducible, surface modified substrates are highly stable and more importantly reusable. The demonstrated method for the alignment of BCLCs advances a step forward towards the realisation of applications proposed for these fascinating compounds.

Keywords: *Flexible polymer substrate, Surface Functionalisation, Bent-core, Nematic, Vertical alignment.*

Anti-oxidant, Anti-inflammatory and Antimicrobial activity of *Nelumbo nucifera (white flower)*

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ABSTRACT

The plant *Nelumbo nucifera* (Lotus plant) is having medicinal importance. The present study was designed to investigate the anti-inflammatory, anti-oxidant and antimicrobial activities of the sample isolated from the ethyl acetate fraction of flowers of *Nelumbo nucifera*. Anti-inflammatory activity of the sample was determined by HRBC membrane stabilization and Albumin denaturation methods. Anti-oxidant activity of the sample was determined by DPPH assay and ABTS method. This compound was shown to possess antimicrobial activity against bacteria and fungi. Four bacterial strains *Salmonella typhi, Escherichia coli, Enterococcus faecalis, Bacillus cereus* and two fungal strains *Curvularia lunata and Candida albicans* were tested by using disc diffusion method. The anti bacterial activity of the compound isolated from ethyl acetate fraction is almost comparable with standard solvent control *Chloramphenicol*. The antifungal activity is almost comparable with standard solvent control *Fluconazole*.

Keywords: *Nelumbo nucifera. Antioxidant activity, Anti-inflammatory activity, Antimicrobial activity, HRBC method, Albumin denaturation, DPPH, ABTS assay, Diffusion method*

Chitosan Coated - Fe_2O_3 Nanopartiles For Dye Adsorption

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ABSTRACT

Chitosan is a promising natural-derived polymer for dye adsorption owing to its rich source, good biodegradablity and high adsorption capacity. To solve the problem, the chitosan doped with Fe_2O_3 nanoparticles (CS-Fe_2O_3 NPs) was successfully prepared via a chemical precipitation method using sodium hydroxide. The synthesized material were characterized by using UV–vis, FTIR, XRD, HR-SEM and BET analysis. The CS-Fe_2O_3 NPs were further applied to remove MB, the effect of pH, initial dye concentration and adsorbent amount of dye adsorbed were investigated using a batch experiment. The pseudo first order and pseudo second order kinetic models were used to describe the kinetic data. It was observed that the pseudo-second-order kinetic model described the adsorption process better than first pseudo-first-order. The Langmuir and Freundlich adsorption model were used for the numerical depiction of equilibrium data, and the best fit was obtained using the Freundlich isotherm model. The CS-Fe_2O_3 NPs demonstrate the virtue of simple fabrication process, high adsorption capacity and good reusability, which is a promising adsorbent for dye removal.

Keywords: Chitosan, Fe_2O_3 NPs, Methylene blue, Langmuir, Freundlich Adsorption

A Facile Synthesis and magnetic characterization of $LaFeO_3$ nanoparticles using Egg white method

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Complementary to Bulk magnetic materials, ferrite materials with nanostructures have received great interest due to their large surface-to-volume ratio and quantum confinement effects. Among the ferrites, Lanthanum ferrite (LFO) shows an excellent improvements in fuel cells, membranes, sensors and electrical devices [1-2]. Here, we report simple technique and cost effective method to synthesize LFO nanoparticles with uniform structure using extracted Egg white method. The phase formation of LFO has been confirmed by powder X-ray Diffraction and RAMAN techniques. As-synthesized product was also subject to TG/DTA analysis to confirm the phase formation. FE-SEM and TEM analysis of sintered nanoparticles show uniform nanostructures. VSM studies, low temperature FC and ZFC measurements were carried out to find the magnetic properties of LFO nanoparticles. From the fig. 1(a), it reveals that crystallite size dependence magnetic behavior was observed. Further, to confirm the magnetic nature of LFO, ESR measurement was also carried out and measured the effective g-factor value of LFO is g = 2.17 at room temperature.

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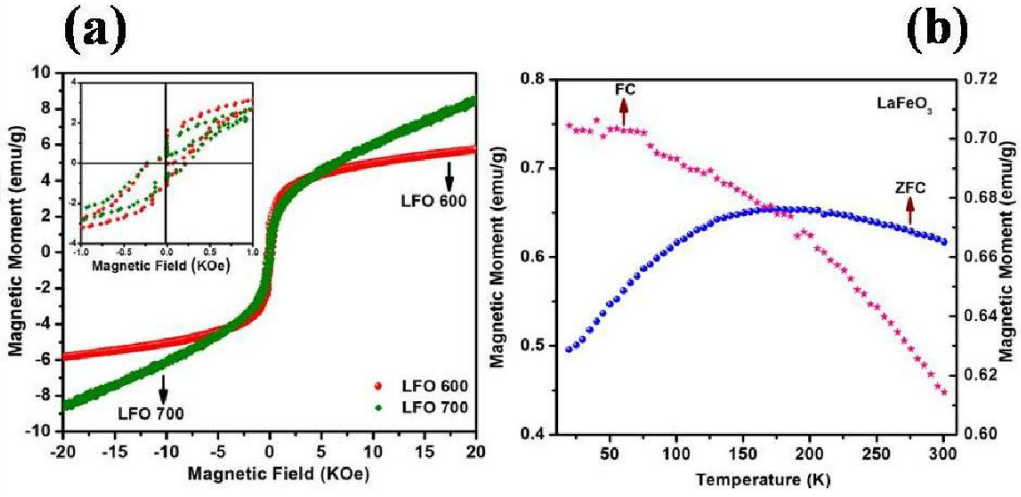

Advanced Nanomaterials in Sustainable energy Development

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The demand of energy has dramatically increased since the start of the industrial revolution, in which the transformation of heat into motion began to be applied. This increase is the result not only of industrial development but also of population growth. Nowadays, the majority of the energy sources are non-renewable, such as fossil fuels coal, oil and natural gas, which provide over 80% of our energy-plus uranium. These sources are contaminating, dangerous, or produce a strong impact on the environment especially the climate; hence, the world is in search of alternative renewable sources of energy.

A novelty of Dye-sensitized solar cell (DSSC) is a potential candidate to replace conventional silicon-based solar cells because of high efficiency, cheap cost and lower energy consumption in comparison with silicon solar panel. In this pape, recent development of component TiO_2(10μm) photoanode, natural dye sensitizer, electrolyte and counter electrode is used to investigate material characteristics, carriers transport, and photovoltaic performance for future DSSC application. The following characterization studies are carried out SEM, XRD, photoluminescence and UV-Visible spectroscopy. Moreover, the origin of the improved performance through electrochemical analysis including cyclic voltammetry and impedance spectroscopy.

Keywords: Nanomaterials, Dye, spectroscopy, impedance, Cyclic Voltammetry

Antimicrobial Screening and spectral study of Mixed Ligand Cadmium complex with Isoniazid and Nitrite

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Abstract

Mixed Ligand Metal complexes (MLMC) of Cadmium were synthesized by using bioactive Isoniazid and nitrite ion as co-ligand. The elemental composition of the synthesized MLMC was measured using Elemental analyzer. MLMC were characterized using various spectroscopic techniques. IR spectroscopy helps to determine the non-bridging nature of the nitrite ligand as well as chelating nature of isoniazid. Nuclear magnetic resonance (NMR) spectroscopy gives the nature of peak environment of organic compounds after coordination. Electron spin resonance spectroscopy (EPR) explains the 'g' value, magnetic nature and coordination mode of the MLMC. The *E-coli* bacteria were used to determine the anti-bacterial activity of synthesized complex. The Cd complex does not support the growth of bacteria. The presence of metal ion was also confirmed by EDAX analysis. The SEM analysis predicts that the cadmium complex exhibits flaky like structure. Electronic spectral transitions reveal the distorted octahedral geometry of the complex.

Keywords: Complex, Isoniazid, Nitrite, antibacterial activity

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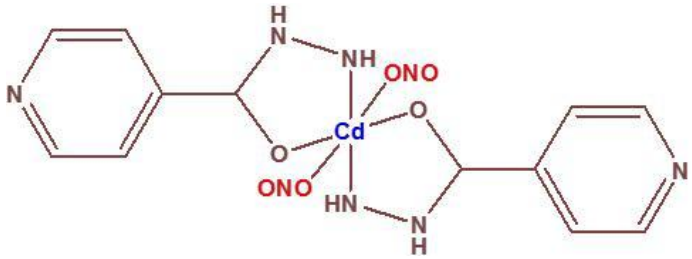

Constructing a novel porous Sulfur-doped g-C_3N_4 hetrojunction nanosheets for highly efficient photoelectrocatalytic environmental remedies

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ABSTRACT

In this work, a novel porous self S-doped graphitic carbon nitride nanosheet (CNS) from a simple dicyandiamide, thiourea and chitosan by a thermal condensation approach in air. Several researchers endeavor to fabricate the exfoliated two dimensional CNS are superior properties to their bulk carbon nitride (CN). Additionally, some of the reports involving construction of iso type hetero junction between two different precursors of a CN enable the formation of an iso type junction at their crystal interfaces can effectively improve the charge driving force. The improvement of charge separation, electron transfer, and specific surface area will achieve simultaneously in such porous S-doped CNS for the first time by combining S doping and thermal exfoliation strategies. The phase and chemical structure, electronic and optical properties of the catalysts will be characterized. The as-prepared catalyst will evaluate by the degradation of both colored and colorless pollutants. The stability and electronic band structures of the catalyst will be analyzed by electrochemical analysis

Keywords: *g-C_3N_4, 2D nanosheets, porous structure, synergistic effect, photoelectrocatalysis*

Exploring the effect of nano-silver concentration on the PEES/ Nano-silver nanfiltration membranes

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Water scarcities problems will very worsen in the future. To supply the fresh water for drinking purposes only the way to treat ground water with low cost membranes. Nano filtration membranes were widely applied to remove arsenic, fluoride and nitrate from ground water. The present study deals with the preparation of nano hybrid membranes based on the different concentration of nano- silver (0 .2 wt%, 0.4 wt%, 0.6 wt%, 0.8 wt%, 1 wt%) and Poly(1,4-phenylene ether-ether-sulfone) were prepared by the Non solvent Induced Phase separation method. The prepared membranes were examined in terms of ATR-FTIR, SEM, AFM, TGA, DSC, hydrophilicity, viscosity, pure water permeability and mechanical properties. The rejection characteristics of arsenic compounds such as As (III) and As (V) were evaluated at pH 3 and 8. The simulated fluoride and nitrate containing water was adjusted to a neutral pH. The NF system obtained fluoride, nitrate and arsenic removal efficiencies of 70~80 % , 50~58 % and 92~99%, respectively, a preferable permeate flux of 175 $Lm^{-2}h^{-1}$, 202 $Lm^{-2}h^{-1}$ and 275 $Lm^{-2}h^{-1}$ respectively. The results revealed that the incorporation of nano silver (0.6 wt %) into PEES hybrid membranes showed better performance compared to pristine PEES nano filtration membranes.

Keywords: *Arsenic, nano silver, PEES, Hybrid membranes*

HIGH DURABILITY OF SPEEK-$BaCeO_3$ NANO COMPOSITE MEMBRANES FOR PEM FUEL CELL APPLICATION

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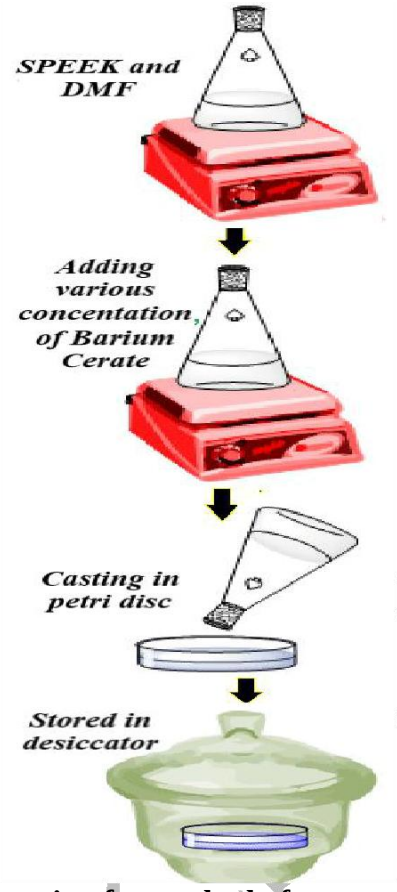
ABSTRACT

Fuel cells have established much attention to generate clean energy production in the field of transportation, portable power systems, and stationary applications etc. Proton exchange membrane fuel cells (PEMFC) have been paying immense interest as new energy conversion technologies. The widespread use of PEMFC for its unique advantages compelled researchers for precise modeling of its characteristics. Herein, perovskite-type $BaCeO_3$ nanoparticles were used for enhancing the properties of sulfonated poly (ether ether ketone) (SPEEK) based PEM. The $BaCeO_3$ nanoparticles were synthesized using co-precipitation method to obtain fine nano scale and submicron oxide powders with a low tendency towards agglomeration. Novel proton conducting nano-composites membranes have been synthesized by various concentrations of $BaCeO_3$ nanopowders grafted into SPEEK matrix by solvent casting technique. The as-prepared membranes were characterized by scans of XRD, FTIR and NMR for the phase and functional group identification. Surface morphology analyses of the membranes were analyzed using SEM and AFM. The thermal stable until 200°C and mechanical analyses confirmed that the nano-composite membrane had improved properties over the pure SPEEK membrane. Other electrochemical and physical properties related to conductivities, water uptake, ion exchange capacity, proton conductivity and durability are also evaluated. Consequently, among all investigated assay proved the membrane samples synthesized 85 wt. % SPEEK/ 15 wt. % $BaCeO_3$ will have a remarkable promising application as an proton exchange membrane for fuel cell.

Key words: SPEEK, perovskite, $BaCeO_3$, solvent casting technique, electrochemical property, PEMFC.



Scheme 1: Pictorial representation for method of preparation of composite membrane

Investigation of electrochemical sensor for dopamine using bienzyme modified electrode

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Abstract

The aim of this work is to study the electrochemical behaviour and the direct electrochemical determination of dopamine by PEDOT-rGO-PPO-LAC (Polyphenol Oxidase-PPO and Laccase-LAC). Advantages of the glassy carbon electrode and the advantages of electrochemical techniques were lead to a low cost, more simplicity and increasing the sensitivity, selectivity and reproducibility of the method. PEDOT-rGO- PPO-LAC film was deposited on a GCE and reduced the graphene oxide by amperometric method. PEDOT-rGO- PPO-LAC was electroactive giving characteristic response at pH 6.0 Cyclic voltammetric studies were carried out for PEDOT-rGO- PPO-LAC at pH 6.0. DPV method was used to study the relationship between response current and dopamine concentration. Linear range obtained for the concentration of dopamine is 5×10^{-8} to 4.6×10^{-5} and the lower limit of determination 8×10^{-9} M. In this modification, the PEDOT-rGO- PPO-LAC has better performance on determination dopamine.

Keywords: *Sensitivity, Dopamine, Amperometric, Differential Pulse Voltammetry, Cyclic Voltammetric.*

Efficiency enhancement of poly (aniline) incorporated with Titanium dioxide (TiO_2)-Nickel oxide (NiO) composite photo-anode for dye sensitized solar cell

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Abstract:

Poly (aniline) (PANI) incorporated with Titanium dioxide (TiO_2)-Nickel oxide (NiO) ternary composites were prepared by a chemical polymerization method. HR-SEM image of PANI-TiO_2-NiO was observed in granular structure based nanowires. The semi-crystalline nature of PANI-TiO_2-NiO was examined by the XRD pattern analysis. The functional group of PANI-TiO_2-NiO was identified that the FT-IR spectroscopy. The absorption maximum of as prepared PANI-TiO_2-NiO was observed in 340 nm and also 2.56 (eV) Optical band gap energy of PANI-TiO_2-NiO was measured by the Tauc plot method. PANI-TiO_2-NiO was achieved that the better electrical conductivity of 3.562×10^{-4} Scm^{-1} by the AC impedance spectroscopy. TiO_2, PANI-TiO_2, TiO_2-NiO, PANI-TiO_2-NiO were used as photo-anode, platinum coated FTO glass plate used as a back electrode. Finally, PANI-TiO_2-NiO was giving 8.73% of power conversion efficiency.

Key words: *Poly (aniline), Titanium dioxide, Nickel oxide, Photo-anode, Dye-sensitized Solar Cell, Efficiency.*

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The SPEEK, PAI and Fe_2TiO_5 acid-base nanocomposite polymer for cations exchange membrane fuel cells.

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Abstract

The sulfonated poly(ether ether ketone) is one most promising aromatic proton exchange polymer membrane concerning fluorinated aliphatic polymer of Nafion in the hydrogen fuel cell. The solvent casting technique is manipulated to achieve the nanocomposite membrane based on the acid (SPEEK)-base (PAI)-inorganic nanoparticles (Fe_2TiO_5) organization. The fabricated proton exchange membrane is examined by the XRD, FTIR, FE-SEM, TGA, oxidative and electrochemical property. The ionic types of acid-base interactions of SPEEK-PAI polymer chain extensively extend the stability criteria such as the thermal, mechanical and diminished the hydrophilic property this delivered to the smaller proton conductivity than SPEEK membrane.To expedite the efficient protons migration in the acid-base polymer of SPEEK-PAI by the adjunct of hydrophilic Fe_2TiO_5 Pseudobrookite nanoparticles in the matrix within the electrostatic polar end of metal-oxide nanoparticles and sulfonic acids of SPEEK. The presence of hydrophilic nanoparticles in the blended membrane lets the more water channels to form the enriched conductivity, water uptake, stability and constrained swelling ration in the elevated temperature. The optimized composition of SPEEK (90 wt%)/PAI (10 wt%)/ Fe_2TiO_5 (6 wt%) secure the highest conductivity of 2.54 mS cm^{-1} at 80˚C and suite for the proton exchange membrane in the fuel cell. The polarization study shows the current density, power density at 80˚C for nanocomposite membrane 284 mA cm^{-2}, 54 mW cm^{-2} in the OCV of 0.92 V.

Keywords: PEMFC, SPEEK, Fe_2TiO_5, PAI, Proton conductivity, Nanocomposite

In Silico Study on Molecular Dynamics Simulation of Self assembled nanoparticles against Chikungunya viral disease

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ABSTRACT

Chikungunya is a mosquito-borne viral disease which is the most significant human viral disease represents a serious public health problem in tropical and subtropical countries of the world. The symptoms of Chikungunya includes sudden onset of fever, severe headache, chills, nausea, vomiting and severe joint pain in the ankles, fingers, toes, elbow, knees and wrists. Most of the patients fully recovered, however in 10 % of the cases are not recovered due to chronic joint pain which may persist for several weeks or months or years together. NSP3 protein is essential for Chikungunya Virus (CHIKV) replication. Similar to other alpha viruses, CHIKV NSP3 not only performs virus RNA replication but is also crucial for other activities, essential for virus infection and pathogenesis. Several chemotherapy drugs are commercially available however they are not effective to cure the disease due to the severe side effects and low drug loading capacity. Combination drug therapy is one of the best therapies to form the self assembled nanoparticles which can deliver by themselves without any carriers. This work is to study the *in silico* approach of molecular dynamic simulation using self assembled nanoparticles with target NSP3 protein. The method can be performed to assess the molecular docking, density functional theory, stability and intermolecular forces, as well as to explain the mechanism between the drugs. The low energy binding mode of the ligand and efficacy were analysed by molecular docking studies based on the score and the interaction of the self assembled nanoparticles with residues were identified. In addition ADME properties of the compound and binding free energy of the complex were analysed which can obey the pharmaceutical relevant parameters. Hence, self assembled nanoparticles show promising inhibitory effect on NSP3 protein.

Keywords*: Chikungunya, CHIKV NSP3 protein, Self assembled nanoparticles, In silico method.*

Development of Novel Self Assembled Amphiphilic Twin Drugs Nanocarriers by using *in silico* approach

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ABSTRACT

Cancer disease is one of the leading cause of death worldwide responsible for 9.6 million death in 2018 which was reported by WHO in the year of 2018. Particularly, breast cancer is a second insidious disease among the causes of cancer deaths of women. The latest cancer statistics estimates, approximately 87,090 women died and every 8 minutes one woman died from breast cancer. Human Epidermal growth factor receptor 2(HER2) is a member of epidermal growth factor receptor family having tyrosine kinase activity. HER2 protein is mainly involved in the over expression and signalling of cell cycle process is a most potential target for breast cancer therapy by preventing cell proliferation activity from the MAPK pathway. Nanoparticles based drug therapy plays a crucial role to increasing a therapeutic efficiency against cancer by establishing the combination of nano material and chemotherapeutic agents. Traditional chemotherapy drugs are often associated with low therapeutic effects and due to the poor pharmacokinetic properties of the drugs used. But the twin drug approach, having greater synergistic efficiency and it can produce more potent pharmacological effects, because the two different pharmacological activities enter into the host cancer cell. In this study, they reveal the potential inhibitor for HER2 protein by performing the molecular docking studies using the amphiphilic twin drug as self assembled nanoparticles. The binding affinity of the protein ligand complex was identified based on the docking score and interaction of residues with twin drug compound. And also performed the ADME/T predictions were used to determine the pharmacokinetic and pharmacodynamic properties of the twin drug. Molecular dynamics simulation study was performed to confirm the efficiency of the twin drug compound against HER2protein.

Keywords: Breast cancer, HER2 protein, Twin drug, Molecular docking, Molecular dynamic simulation.

Synthesis, Characterization and Biomedical Application of MgO Nanoparticles

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ABSTRACT

Magnesium oxide nanoparticles (MgO NPs) were synthesized by using Magnesium chloride hexahydrate and Sodium hydroxide. UV-Visible diffuse reflectance spectroscopy and X-ray diffraction were used to confirm the synthesized sample. FT IR spectra were carried out to know the changes in the functional group of the product by comparing with the reactant. High-resolution transmission electron microscopy (HR-TEM) and high-resolution scanning electron microscopy (HR-SEM) were assisted to investigate the morphology and size of the synthesized sample. These morphologies show that the synthesized sample had sphere-like morphology. The elemental composition of the MgO NPs was determined by energy dispersive X-ray analysis (EDX). Cytotoxicity studies were carried out and showed better performance for the synthesized MgO NPs.

Key words: *Magnesium Oxide, Nanoparticles, Electron microscopy, Cytotoxicity.*

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Comparative study on Physico-Chemical properties of Green grapes (vitis vinifera) and Panneer gapes.

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Abstract

Juice can be considered as an important and functional ingredient in food products. It is a good source of Vitamin-A, Vitamin-E Vitamin-B_6, thiamin, calcium and potassium Bergamottin, an active compound –that occurs naturally in grape fruit, has been showen to protect against due to its anti oxidant, anti-inflammable, antitumor properties. According to 2015 review published in the international journal of molecular sciences. This substance is appears to be particularly effective in the prevention and treatment of lung, breast and skin cancers, leukemia, myeloma and more Bergamottin inhibits tumour growth and stops cancer cells from spreading throughout the while reducing inflammation. 2017 review suggest that grapefruits are linked to the decrease in systolyic blood pressure.

The aim of the present study was to analyse and compare the Physico-Chemical properties of green grapes and panneer grapes. The fruits were collected washed and fruits juice was prepared and Physico-Chemical properties were analysed.

The pH of the juice found in the range 2.7 (green grapes) and 3.0 (panneer grapes).The reducing sugar analysis showed that the panneer grapes the higher content of reducing sugar (6.2g) than panneer grapes (2.941g).the predominant acid present in grapes is tartaric acid. The total titrable acidity found to be 0.7725% for green grapes and 0.555% for panneer grapes.

Key words: *green grapes, panneer grapes pH, Titrable acidity.*

Analysis on Physico-Chemical properties of Sweet orange (kodai) and Citrus limetta (Sathugudi)

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Abstract:

Citrus fruits are an excellent source of vitamin-C, A nutrient that strengthens the immune system and keeps your skin smooth and elastic. Orange has all the Vitamin-C need in a day. Citrus fruits are a good source of fiber, eating Citrus fruits could be good for your heart. In fact, Japanese study found that people who ate higher amounts of Citrus fruits had lower rates of heart diseases and stroke.Flavonoids found in Citrus fruits have anti-inflammatory capabilities that are thought to help protect against the chain elements that cause the Nervous system to deteriorate. Orange juice contains lots of Vitamin and other nutrients.

The aim of the present study was to analyse and compare the Physico-Chemical properties of Sweet orange (kodai) and Citrus limetta (Sathugudi).The fruits were collected, washed, crushed and fruit juice was prepared and Physico-Chemical properties were evaluated.

The pH of the juice found in the range 3.0 Sweet orange (kodai) and 3.1 Citrus limetta (Sathugudi).The reducing sugar analysis showed that than Citrus limetta (Sathugudi) has higher content than Sweet orange (kodai). The predominant acid present in Orange is citric acid. The total titrable acidity is showed that Sweet orange (kodai) has higher titrable acidity that Citrus limetta (Sathugudi).

Key words: *Sweet orange, citrus limetta, pH, Titrable acidity.*

MICRO-CRYSTALLINE CELLULOSE DISPERSED POLY (VINYL ALCOHOL) FILM FOR FOOD PACKAGING APPLICATIONS

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Abstract

In the present work, the microcrystalline cellulose was synthesized by the jute fiber and was identified by Scanning electron microscopy. The synthesized microcrystalline cellulose was dispersed into the poly (vinyl alcohol) by simple ultra-sonication process and evenly coated into the food packaging sheets. The surface morphology of the synthesized microcrystalline cellulose dispersed poly (vinyl alcohol) film was studied by Scanning electron microscopy. The crystalline nature of the microcrystalline cellulose dispersed poly (vinyl alcohol) film was characterized by X-ray diffraction. The thermal properties of the synthesized microcrystalline cellulose dispersed poly (vinyl alcohol) film were investigated by Thermogravimetric analysis and Differential Scanning Calorimetry. The prepared microcrystalline cellulose dispersed poly (vinyl alcohol) film as a promising candidate for food packaging applications.

Keywords: *Micro-crystalline cellulose, Poly (vinyl alcohol), Food packaging applications, Ultra-sonication*

Exploration of High Performance $MnSn(OH)_6$ Electrodes for Energy Applications

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Abstract

A successful attempt for producing $MnSn(OH)_6$ high performance electrodes for energy applications has been reported in this work. Solvothermal processing route was tuned to produce $MnSn(OH)_6$ uniform nanocubes was adapted. Single phase tetragonal $MnSn(OH)_6$ nanocubes were validated by XRD study from the sharp diffraction peak of crystal plane (200). Intrinsic phonon vibration of tetragonal $MnSn(OH)_6$ nanocubes were confirmed by Raman spectra. Interaction with photons and emissive nature of nanocubes were deliberated by PL spectra for the excitation wavelength of 300 nm. The characteristic Mn-O, Sn-O and OH vibrations of $MnSn(OH)_6$ nanocubes were evaluated by FTIR spectra. Uniform nanocube formation and its dispersive nature were extensively examined by SEM images. Fabrication of scalable high performance $MnSn(OH)_6$ electrodes achieved by standard coating method. The fabricated $MnSn(OH)_6$ nanocube electrodes systematically analyzed in Biologic SSP 150 work station at room temperature to evaluate its electrochemical performance for energy applications. The highest specific capacitance of 525 F/g at 5 mV/s achieved for uniform nanocube morphology of $MnSn(OH)_6$ electrode. The water oxidation nature of the mentioned electrode yielded outstanding result of LSV study as 288 mA/g for 10 mV/s scan rate whose electrical conductivity, electron mobility and charge transfer kinetics were investigated by EIS spectra from 100mHz to 100kHz frequency range and also the superior stability over 24 h of electrochemical OER activity also proposed. Hence, the high performance $MnSn(OH)_6$ nanocube synthesis and fabrication was achieved for energy applications such as super capacitors and water splitting.

Keywords: *$MnSn(OH)_6$ Nanocubes; Super capacitor; Water splitting.*

Fabrication of Efficient Hydroxide based Cobalt Tin Binary Metal Electrodes for Electrochemical Applications

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Abstract

In this work, Cobalt tin hydroxide ($CoSn(OH)_6$) nanoparticles were prepared by using hydrothermal optimization process. Role of precipitating agent concentration on physical, morphological and electrochemical properties of $CoSn(OH)_6$ was studied thoroughly. Cubic $CoSn(OH)_6$ phase was confirmed by the resolved diffraction peak at 22.8^o of (200) crystal plane by XRD spectra. The characteristic Raman and FTIR active modes of cubic phase $CoSn(OH)_6$ nanoparticles have been analyzed. Electron recombination and trapping under excitation of 300 nm was intensively studied by PL spectra. Morphological variations and dispersive nature of $CoSn(OH)_6$ nanoparticles with respect to the precipitating agent concentration was investigated from SEM images and also the band gap estimations based on particle size effect was revealed by UV spectra. Complete investigation of electrochemical activity of fabricated $CoSn(OH)_6$ electrodes and the electrochemical mechanism of hydroxide based cobalt tin binary metal electrodes for electrochemical applications has been proposed with the help of CV, LSV, EIS and CA studies. As per the electrochemical analysis of fabricated electrodes, efficiently performed $CoSn(OH)_6$ nanoparticles synthesized by higher concentration of precipitating agent exhibited 495 F/g at 5 mV/s scan rate with higher electronic mobility. The water oxidation reaction of the same electrode was revealed as 264 mA/g at 10 mV/s scan rate. The long time OER activity for 24 h also provided for the efficient $CoSn(OH)_6$ electrode. Since, the studies suggested that the electrochemical performance of fabricated hydroxide based cobalt tin binary metal electrodes may utilize as an efficient electrode for both super capacitor and water splitting applications.

Keywords: *Hydrothermal; $CoSn(OH)_6$; Electrochemical mechanism.*

Investigation of layered $NaNi_{5/10}Ti_{3/10}Mg_{2/10}O_2$ anode material for secondary Na-ion batteries

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Abstract

Sodium-ion batteries are significant alternative energy storage device that have recently come again into focus for the development of large-scale energy storage devices, because sodium is an earth abundant and low-cost material. In this article, we report that the layered $NaNi_{5/10}Ti_{3/10}Mg_{2/10}O_2$ anode material has been successfully prepared via solid stated reaction. The as-prepared material was characterized by TG, XRD, FTIR, SEM and XPS. The calcination temperature of the anode material was confirmed through the TG analysis. The monoclinic structure with the space group of C2/m of prepared material has been determined from XRD analysis. The functional group vibration of the prepared material studied using FT-IR. XPS spectra suggest that Ni, Ti and Mg are present in +2, +4 and +2 oxidation states, respectively. SEM analysis confirmed that hexagonal plate-like particles are appeared in the sample. Therefore layered $NaNi_{5/10}Ti_{3/10}Mg_{2/10}O_2$ anode material may be a suitable for Na-ion batteries.

Keywords: *Solid State reaction, anode material, layered structure.*

Sepiolite wrapped sulfur/ ZrO_2 twofold merged cathode material for Li-S battery

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Abstract

Modern energy societies have tremendous developments in the area of energy storage devices, due to the augmentation of fossil fuels need and the pollution existence. Lithium-sulfur (Li-S) batteries have become powerful competitor for the next-generation of high energy secondary rechargeable batteries. Li-S battery can produce much more attentiveness for attaining high energy density, good protection and low cost. This system endures several drawbacks: low electric/ionic conductivity, high dissolution of polysulfides and the volume expansion of sulfur. To overcome these shortfalls, the selected additives were added in to the electrode material during the preparation. Herein, we used sieved sepiolite has been preferred as an additive material to list upon the above challenges in sulfur battery. The S/PTSep/ZrO_2 nano material has been prepared by simple heat treatment method. The as-prepared samples have been characterized by XRD, FTIR, RAMAN, SEM with EDAX and TEM analyses. The morphologies of SEM images show that the particles have erratically various sizes of unflustered porous particles detached in the nano-matrix with agglomeration. In summary, Li-S cells can be estimated to proficiently improve the consumption of sulfur and restrain the dissolution of polysulfides into electrolyte.

Keywords: *Energy storage, ZrO_2 nanoparticles, polysulfide dissolution, electrolyte.*

Structural analysis of layered O3-type $NaFe_{0.7}Ti_{0.2}Cr_{0.1}O_2$ cathode material for sodium ion batteries

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Abstract

Sodium-ion batteries (SIBs) have attracted broad interest in large-scale energy storage applications for renewable energy and smart grid, due to abundant sodium resources and low cost. O3-type layered sodium transition metal oxides (i.e., $NaMO_2$, M=Ti, V, Cr, Mn, Fe, Co, Ni, Cu, etc.) are considered as the propitious class of cathode materials for SIBs due to their high capacity and easy to synthesis. In this work, the layered O3-type $NaFe_{0.7}Ti_{0.2}Cr_{0.1}O_2$ cathode material was successfully prepared via solid stated reaction. The as-prepared material was characterized by Thermo gravimetric analysis, X-ray diffraction, Fourier transform infrared spectroscopy, Scanning electron microscope and X-ray photoelectron spectroscopy. The calcination temperature of the cathode material was deep-rooted through the TG analysis. The XRD pattern was indexed to a rhombohedral structure with the space group of R$\bar{3}$m. The presence of Na -O bond was confirmed by FTIR spectra. From XPS analysis, the presence of Fe, Ti and Cr ions occurs in +3, +4 and +3 oxidations states respectively. SEM results revealed the morphology of the material. Hence, the layered O3-type $NaFe_{0.7}Ti_{0.2}Cr_{0.1}O_2$ may be a favorable cathode material for sodium ion batteries.

Keywords: *Solid State reaction,* $NaFe_{0.7}Ti_{0.2}Cr_{0.1}O_2$*, Cathode material, O3-type.*

SPECTRAL AND OPTICAL PROPERTIES OF 2-AMINOPYRIDINIUM p-HYDROXYBENZOATE NONLINEAR OPTICAL SINGLE CRYSTAL

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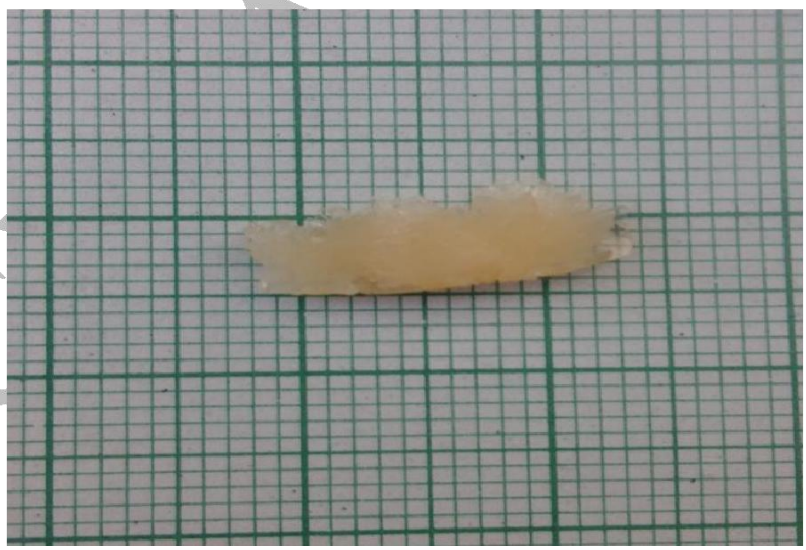
ABSTRACT:

2-aminopyridinium p-hydroxybenzoate (2APH), an organic optical single crystal has been synthesized using slow evaporation solution growth technique at ambient temperature. The crystal structure, space group and lattice parameters were determined by single crystal x-ray diffraction studies. The powder x-ray diffraction analysis confirms the crystalline nature of 2APH crystal and the (hkl) values were indexed. FT-IR spectroscopy was used to confirm the presence of various functional groups in the compound. The UV-VIS transmission spectrum of 2APH in the range of 200-1000 nm shows lower cut-off wavelength at 320 nm was estimated from the optical studies. The photoluminescence spectrum showed violet emission peak at 360 nm .The thermal stability of the grown crystal was evaluated using thermogravimetric and differential scanning analysis. The second harmonic generation (SHG) efficiency was estimated using the Kurtz–Perry powder test.



SYNTHESIS, GROWTH, STRUCTURAL AND OPTICAL PROPERTIES OF 8-HYDROXYQUINOLIUM MYRISTATE NONLINEAR OPTICAL SINGLE CRYSTAL

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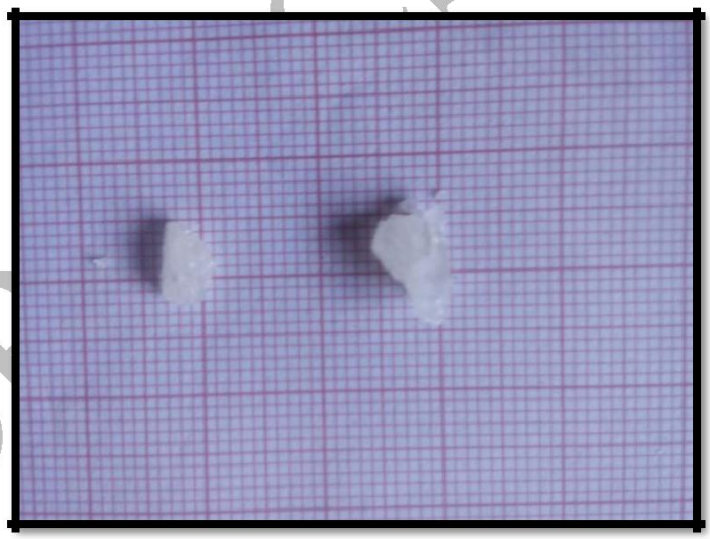
ABSTRACT:

The 8-hydroxyquinolium myristate (8HMY) organic nonlinear optical single crystal was grown by slow evaporation solution growth method using water as a solvent. The single crystal X-Ray diffraction studies confirmed that the 8HMY crystal belongs to monoclinic structure with centrosymmetric space group P. The crystalline perfection was confirmed by powder X-ray diffraction analysis. The chemical composition and functional group of the 8HMY were confirmed by the FT-IR and Laser Raman spectroscopy analysis. The optical absorption spectrum having the cut-off wavelength at 378 nm and band-gap energy was found to be 4.15eV. PL spectral study of grown 8HMY showed an high intense emission peak at 470 nm for an excitation wavelength at 382 nm. Thermal stability of the material is confirmed by the thermal analysis. Nonlinear optical studies confirmed by the Kurtz-Perry powder SHG test.



Photograph of grown crystal 8HMY

STUDIES ON THE SPECTRAL AND OPTICAL PROPERTIES OF ORGANIC NON-LINEAR OPTICAL 2-AMINOPYRIDINIUM 5-CHLOROSALICYLATE SINGLE CRYSTAL

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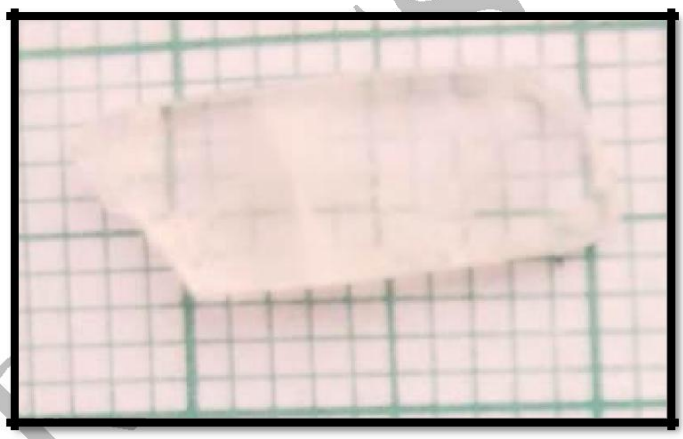
Abstract

Organic nonlinear single crystal of 2-aminopyridinium 5-Chlorosalicylate has been grown by slow evaporation solution growth method at room temperature using as ethanol: water mixed solvent. The crystal system, space group, various planes of reflections and crystal perfections were identified by single crystal and powder X-ray diffraction analyses. FT-IR and FT-RAMAN spectral studies have been performed to various functional groups present in the compound. Optical transmittance of the grown crystal (2A5C) has been studied by UV-VIS spectrum. The energy band gap of the material is found using tauc's plot and by direct method. UV–VIS transmission studies revealed that the grown crystal was optically transparent through visible range making it suitable for NLO applications. Photoluminescence spectrum showed sharp, well defined emission peak at 416 nm.The thermal stability and decomposition stages were analyzed through TG-DSC techniques. The Kurtz-perry powder second harmonic generation technique confirms the nonlinear optical property of the grown crystal.



Photograph of as grown 2A5C crystal

CHITOSAN – PVA –COMPOSITE FILM FOR WOUND HEALING

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The present study reports the preparation of Chitosan – PVA Film for Wound healing. Chitosan – PVA scaffold was prepared by solvent evaporation method. Chitosan was extracted from powdered crab shells upon various chemical treatments. PVA composite film were prepared by the reinforcement of the extracted chitosan (3 wt %) into the PVA (10 wt %) matrix and subsequent film casting. The morphology, diameter and structure of the prepared Chitosan – PVA composite film were studied by scanning electron microscope(SEM). The average particle size of the extracted chitosan was found to be 43nm. The thermal properties of films were studied by TGA analysis. The Chitosan – PVA film was immersed in phosphate buffered saline (pH = 7.4) to determine the swelling rate of the scaffold. The Chitosan – PVA patches were placed on the wound cells and tested for wound healing applications. The Chitosan – PVA film healed the wounds faster by providing a good platform for cell repair and growth. The Chitosan – PVA film was found to heal the wound faster than the native chitosan and PVA films.

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Keywords: Chitosan, PVA, polymer composite, wound healing.

Anticorrosive Activity of Copper in Neem Based Biodiesel Using Natural Inhibitor *Syzygium cumini*

P. Indra Priyatharesini

***Abstract* :**

Syzygium cumini seed extract was investigated as a corrosion inhibitor for copper in biodiesel. Inhibition efficiency and corrosion rate were evaluated with different acid values and temperatures. The inhibition efficiency was found to be above ninety percentages for copper in neem oil based biodiesel. The values of free energy of adsorption and heat of adsorption obtained were negative revealing the spontaneity of adsorption of inhibitors on metal surface. Infrared spectral studies revealed the mechanism of corrosion inhibition. Scanning electron microscopy technique revealed the protective attributes of the natural inhibitor. The fuel performance test and emission characteristics of biodiesel were compared in the presence and absence of corrosion inhibitor. The brake thermal efficiency of neem based biodiesel with diesel is lower than diesel and brake specific energy consumption was found to be higher. However, Hydrocarbons, CO and CO_2 and smoke were found to be lower with neem based biodiesel fuel. NOx emissions of neem based biodiesel is found to be little higher that of Diesel. The addition of corrosion inhibitor does not affect the fuel performance of biodiesel. The results from the experiments suggest that biodiesel derived from non-edible oil like neem could be a used as a good substitute to diesel fuel in diesel engine in the near future particularly for the localized energy production. The investigation revealed that neem based biodiesel could be used in conventional diesel engine.

Key Words - Neem biodiesel, Copper, Weight loss measurements, Corrosion thermodynamics, Green corrosion inhibitor, Fuel performance, emission.

Cytotoxicity and Antimicrobial Activities of Copper Nanoparticles Synthesized Using Mimosa Pudica

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ABSTRACT

The present study was to evaluate the biological activity of copper nanoparticles synthesized using ethanolic extract of Mimosa pudica. The plant has been used traditionally for ages, in the treatment of urogenital disorders, piles, dysentery, sinus, and also applied on wounds. In current study, ethanolic extract of Mimosa pudica was used for the synthesis of copper nanoparticles. The formation of copper nanoparticle was confirmed by UV-Visible spectroscopy. Fourier Transform Infra red Spectroscopy (FTIR) revealed the possible involvement of photo-constituents in copper nanoparticles of crude extract.XRD is commonly used to determine the chemical composition and crystal structure of a material. Further Transmission Electron Microscopy (TEM) was used for the shape and morphology determination. The bio- synthesized copper nanoparticles were found to be effective against pathogenic bacterial and fungal strains. The in-vitro cytotoxicity activity of copper nanoparticles was performed against MCF-7cell line (breast cancer cell line) and compared against the vero cell line (normal cell line).The result showed that the copper nano particles show moderate activity against the cancer cell but seems to have less toxicity towards normal cell.

KEYWORDS: *Copper nanoparticles, mimosa pudica, UV-Visible, FTIR, XRD, TEM, bacterial, fungal and in-vitro cytotoxicity.*

PHYSICO-CHEMICAL INVESTIGATION OF MANNICH MODIFIED CURCUMIN-SCHIFF BASE COPPER COMPLEX

S. Tamijselvy and P. Andal

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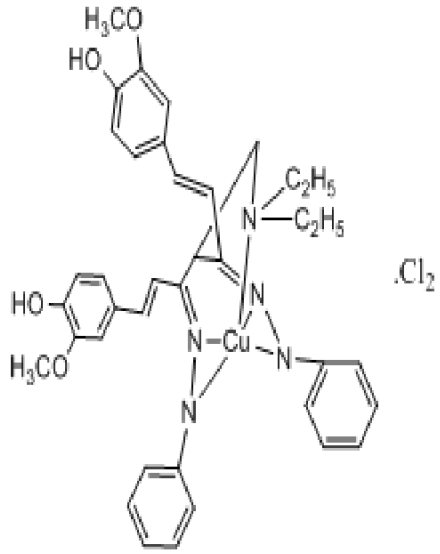
Curcumin has demonstrated both anticancer and anti-angiogenic properties. The anti-angiogenesis effect of curcumin include the inhibition of vascular endothelial cells proliferation in vitro and capillary tube formation and growth in vivo.

The work involves the activation of curcumin by making carbonyl group easily prone to Schiff's reaction. This is done by by Mannich base reaction. It is then made to undergo schiffs condensation and followed by copper insertion. The synthesized molecule is characterized by IR, UV, Mass. The complex shows greater antibacterial and anti-fungal activity when compared to curcumin.



SYNTHESIS OF GRAPHENE OXIDE SUPPORTED WITH BIMETALLIC NANOPARTICLES AND ITS APPLICATION.

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ABSTRACT:

A nanoparticle is a infinitesimal molecules with at least one aspects less than 100 nm. Nanoparticle has immense assortment of prospective applications in biomedical, optical, and electronic fields. Nanoparticles are of great technological fascination as they are effectively a aqueduct between bulk substances and atomic or molecular structures. The properties of matter change as their size approaches the nanoscale and as the percentage of atoms at the surface of a material becomes significant. For bulk materials larger than one micrometre the rate of particles at the surface is minute relative to the total number of particles of the material. The absorbing and occasionally unpredicated properties of nanoparticles are not partly due to the characteristic of the surface of the material dominating the properties in instead of the bulk properties. In this study two different types of graphene oxide supported two mono Ni Mn and a bimetallic Ni\Mn nanoparticles catalyst were synthesized. The size and shape of the products were characterized by various techniques such as : scanning electron microscopy (SEM), x-ray diffraction spectroscopy (XRD). Results proved that the newly developed graphene oxide carried Nickel Manganese nanoparticles catalysts can be more efficient to reductive, oxidative and of environmentally important organic pollutant additionally it is also very good biologically active compound.

Keywords: GO, Ni,Mn, Rhodamine,nanoparticles

Synthesis of Trispiropyrrolidines via Green multicomponent methodology

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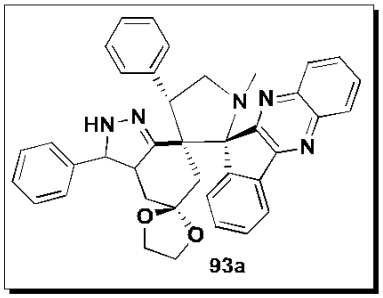
Abstract



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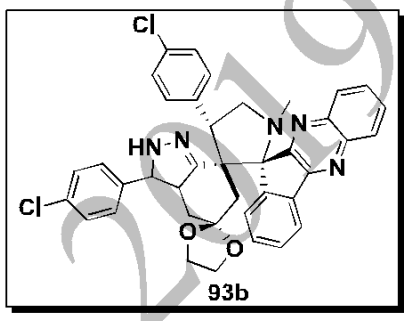

93b

We have carried out 1,3-dipolar cycloaddition reaction of azomethine ylide generated from *o*-phenylene diamine, Sarcosine and ninhydrin with substituted 7,9-bis [(*E*)-arylidene]-1,4-dioxo- spiro [4,5]-decane-8-ones as dipolarophiles in a one pot multicomponent reaction using ionic liquid. When the reaction was carried out in refluxing ionic liquid /methanol a series of novel trispirocycloadducts were formed in good yields. The reaction had occurred by the 1,3-dipolar cycloaddition reaction of azomethine ylide generated from ninhydrin , 1,2-phenylenediammine and sarcosine across the *exo* cyclic double bond of 7,9-bis [(*E*)- arylidene]-1,4-dioxo- spiro [4,5]-decane-8-ones to give Trispiropyrrolidines in good yield.

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A Study on the removal of Methyl Violet Dye using a Low Cost Activated Carbon by Adsorption

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Abstract:

The aim of the present work is examination of Pisonia Alba as Low cost adsorbent material of removal of Methyl Violet from Industrial waste water. Batch experiments were conducted to obtain optimum removal conditions such as concentration of dye, adsorbent dosage and pH of dye solution. The results show higher efficiency of removal of methyl violet from industrial waste water is 89%. Spectroscopic analyses involving FT-IR spectroscopy and Scanning Electron Microscopy were performed to have a better understanding on the mechanism.

Keywords: Low Cost Activated Carbon, Pisonia Alba, Methyl Violet, FT-IR spectroscopy.

Graphene-Based Nanocomposite Photocatalysts for Hydrogen Generation

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Abstract

Hydrogen production from solar water splitting has been considered as an ultimate solution to global energy and environmental issues. Graphene-based photocatalysts have gained increasing interest as a viable alternate to increase photocatalytic H_2 production performance in converting solar energy into chemical energy. The use of graphene to enhance the efficiency of photocatalysts has been proved due to its unique two-dimensional conjugated structure and electronic properties. We synthesized a graphene-$Ni_2Co_3O_4$ oxide nanocomposite by microwave assisted solvothermal reduction of graphene oxide in the presence of Ni and Co precursors. The structural and optical properties of the photocatalysts were studied by XRD, Raman, FESEM and UV-Vis DRS respectively. The photocatalytic activity of the nanocomposite was quantised by degrading the organic dye methylene blue. The nanocomposite exhibiting a bandgap of 2.8 eV exhibit excellent visible light photoactivity.

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CARDANOL PENDENT AROMATIC DIAMINE END CAPPED IMINE SKELETAL NANOSILICA REINFORCED POLOYIMIDE (*n* SiO_2/PI) NANO COMPOSITES FROM CASHEW NUT WASTES

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Abstract:

A novel cardinal pendant aromatic diamine end capped imine skeletal nano silica /polyimide (n SiO_2/PI) nano composite was designed and developed via thermal imidization and poly condensation reactions. The polyimide monomer is prepared from aromatic diamine and pyromellitic dianhydride,which then undergoes polymerization to form polyimide nano composites reinforced with varying percentages of n SiO_2 .The synthesised PI nano composites were characterised by FT-IR. The PI nano composites have shown high thermal stability, good chemical resistance, and low di-electric constant. The incorporated n SiO_2 particles decreases thermal degradation .The air imported by the n SiO_2 plays a crucial role in reducing the dielectric constant.The morphology of PI nanocomposites is evidenced by SEM and AFM images.

Keywords: *Polyimide, thermal imidization temperature, nano silica, PI nano composites,thermal stability and morphological properties..*

SOURCES EFFECTS AND REMEDIAL OF TOXIC METALS IN INTRUSTIAL WASTE WATER

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Abstract

Cadmium, Chromium, Copper, Iron, Zinc, Nickel and Mercury metals were listed as toxic heavy metals which are exist in the various industrial waste water. Sources are for Cadmium launderettes, electroplating workshop, plastic manufacturing, pigments, enamels, paints. For Chromium Alloys, preservatives, dyeing and tanning activities, metal coatings. For Copper Electronics, plating, electrical wires, paper, textiles, rubber, printing, plastic. For Iron Galvanizing, electroplating, polishing. For lead Fuel additive, batteries, pigments, roofing, fishing weights. For Zinc Domestic wastes, galvanizing, batteries, paints, fungicides, textiles, cosmetics, pulp, paper mills, and pharmaceutics. For Nickel Alloys, electroplating, nickel-cadmium batteries, launderettes, paints and for Mercury Dental practices, clinical thermometers, glass mirrors. This toxic metals causes serious health hazards. Cd causes Kidney damage, skeletal damage, itai-itai (ouch-ouch) diseases, and cancer. Zn causes Its deficiency can lead to poor wound healing, reduced work capacity of respiratory muscles, immune dysfunction, anorexia, diarrhea, hair loss, dermatitis and anemia. Pb causes headache, irritability, abdominal pain, nerve damages, kidney damage, blood pressure, lung and stomach cancer and glimas, for children, behavioral disturbance, memory deterioration, reduces ability to under-stand and anemia. These heavy metals in the industrial waste water can be minimized by the following techniques adsorption, biosorption, precipitation reverse osmosis, electrolytic recovery techniques, and liquid–liquid extraction etc. Hence It is very essential to minimize the toxic metal level in the industrial waste water before discharge into the near water bodies.

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