ONE DAY NATIONAL SEMINAR
ON
PROSPECTS IN MATERIAL SCIENCE
26th Feb - 2019

Organized by
PG Department of Physics
Vellalar College for Women (Autonomous)
Erode - 12, Tamil Nadu

NSPMS2019
ABSTRACTS

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National Seminar
on
Prospects in Material Science

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Organized by

PG DEPARTMENT OF PHYSICS
Vellalar College for Women (Autonomous)
Erode-12
Tamilnadu

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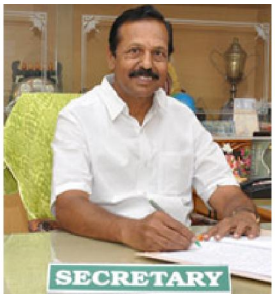

Message

It gives me an immense pleasure in writing this foreward for the Proceedings of the 'One Day National Seminar on Prospects in Material Science', being organized by the PG Department of Physics on February 26, 2019. I am pleased to note that researchers from various Institutes/Universities from different parts of the country are presenting their research papers on the current aspects of Nanotechnology and Material Science.

This event is targeted towards researchers, professionals, educators and students to share innovative ideas, issues, recent trends and future directions in the field of Nanotechnology and Material Science. Seminars like these provide an ideal platform for the confluence of learned minds when knowledge is shared for the benefit of everybody. I am sure that all the delegates would be greatly benefited by the deliberations.

I wish all the participants and delegates a great success in their mission!!

SECRETARY
VELLALAR COLLEGE FOR WOMEN
(AUTONOMOUS)
ERODE - 12.

Dr.N.Maragatham
Principal
Vellalar College for Women
Erode – 638 012

Message

I am extremely happy that PG Department of Physics has organized a 'One Day National Seminar on Prospects in Material Science' on 26th February 2019. This seminar will focus on the recent advances in the field of Nanotechnology and Material Science. Advancement in understanding of a material type is often the forerunner to the stepwise progression of a technology. Hope, a number of delegates from across the country will gather to deliver the invited talks and to present their research papers.

I am confident that, this seminar will definitely provide an interactive platform where scholars, students from various Institutions, Research Laboratories and Industries can meet, discuss and project a road map for materials science research towards novel applications in various fields.

I hereby congratulate the organizing committee members for their efforts to organize a National Seminar. I strongly believe that this endeavour will prosper now and in the years to come.

I take this opportunity to wish a grand success of this National Seminar.

PRINCIPAL
VELLALAR COLLEGE FOR WOMEN
(AUTONOMOUS)
ERODE - 12.

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Message

I am glad to invite all the delegates to a 'One Day National Seminar on Prospects in Material Science' organized by the PG Department of Physics on February 26, 2019. The objective of this conference is to bring the students, researchers and scientists from across the nation on a common platform to share and access the recent trends in the field of Nanotechnology and Material Science and to discuss ways to promote promising societal applications. This seminar is aimed to bring up substantial discussion on major sectors of material processing, characterization and device fabrication to meet the rapid advances in engineering and technology, the globalization and the changing social needs.

60 papers have been selected after peer review by covering wide areas of research in Nanotechnology and Material Science which have been included in the proceedings. I hope this conference would also provide young researchers, engineers, scientists and students an opportunity for interaction and benefiting from each other's wisdom and experience.

I encourage the delegates to take full advantage of the program and tackle the challenges in their respective areas of research.

I thank our Institution wholeheartedly for supporting this seminar.

I look forward all the delegates for their active participation.

Yours sincerely,

(N.Dhachanamoorthi)

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22.02.2019

Message

I am glad to note that One Day **National Seminar on Prospects in Material Science** (NSPMS-2019) is organized by the PG Department of Physics, **Vellalar college for women** on February, 26th, 2019.

The advancements of new technologies are largely based on the development of new materials with unprecedented properties. A seminar on the prospects in materials science will undoubtedly be of current interest and benefit the student community at large.

I am certain that NSPMS-2019 will provide a vibrant platform for productive discussions and will motivate the young minds to forge ahead in the developments of advanced materials. I congratulate the organizers for their commendable efforts and wish the conference a grand success.

22/2/2019

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Date: 19. 02. 2019

MESSAGE

I am quite happy to know that the Department of Physics of Vellalar College for Women, Erode is conducting One Day National Seminar on Prospects in Material Science on 26th Feb-2019. I hope that there will be deliberations enough to highlight the major thrust areas in the field.

With best wishes

Dr. R. K. Biju

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Dr. A. David Stephen. M.Sc., Ph.D
Assistant Professor (S)
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Welcome to the One Day National Seminar on Prospects in Material Science (NSPMS 2019), which takes place in Vellalar College for Women, Erode on February 26, 2019. It has been a real honour and privilege to serve as the resource person of the seminar.

The goal of this event is to bring together the technologies and researchers who share interest in *Material Science*. Its purpose is to promote discussions of research and relevant activities in the design of new materials. Also, this seminar aims at increasing the synergy between academic and industry professionals working in this area.

Ultimately, the NSPMS 2019 program provides international forums for scientists and scholars from academia and industry to exchange and share their experiences, research results, and new ideas on hot and emerging topics on this field.

Yours sincerely,

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The research areas chosen for the seminar is of great value in the present contest. I am sure that it would be unique opportunity for the budding scientist to learn the novel ideas on potential areas of Physics and Technology.

This inciative step will encourage the students to choose their future perspective and so I extend my warm greetings to the organizers.

With my best wishes and personal regards,

Yours sincerely,

(Matheswaran)

Nuclear Shell and Structure Studies via Cluster Radioactivity in the SHE

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Abstract

Super heavy elements are produced by bombarding a target of sufficiently high atomic number with the beam of heavy ions. Successful synthesis of super heavy elements up to 118 has already done by many researchers. Elements with Z>118 is not quite evident, still the attempt to produce Z=120 are reported. The main experimental difficulty for the synthesis of new super heavy element is its reduced probability of formation and separation of compound nuclei from the very high beam of incident projectile nuclei.

The phenomenon of spontaneous emission of particles heavier than the alpha particle by radioactive nuclei is known as cluster radioactivity; it is not an isolated phenomenon and must be related to other processes such as cold fission and cold fusion. This process can be treated as a case of strong asymmetric fission or a decay process of cluster formation and tunneling through the barrier making many assaults on it similar to alpha decay. This phenomenon was experimentally confirmed in 1984 by Rose and Jones and a few months later, Alexandrov et al confirmed this phenomenon in the radioactive decay of ^{14}C from ^{223}Ra.

In the present paper we would like to present the nuclear shell and structure studies through alpha and cluster decay in the super heavy region. The existence of long lived super heavy nuclei is mainly controlled by spontaneous fission and alpha decay process. But many of the elements in super heavy region can be identified via the alpha decay chain. Alpha decay in super heavy nuclei is possible if the shell effects supplies the extra binding energy and increases the barrier height of fission. So the study of the alpha decay from various super heavy elements helps to identify the stability of the parent nuclei.

Cluster radioactivity is also a dominant mode of decay in the super heavy region. In many of our papers, we examined the possibility of cluster emission from nuclei in the super heavy region using Coulomb and Proximity Potential Model (CPPM) as interacting barrier to find the next neutron and proton shell closures in this region and it was found that next neutron shell

closures occur at N= 162,172, 184and 192 and the proton shell closures are at Z=114,120 and 126 which was in confirmation with the other studies.

Beta decay is another decay mode for the nuclei lie beyond the beta stability line. Beta decay process is slow and less favored because it proceeds via weak interaction. For beta decay process the energy released is less compared to alpha decay and spontaneous fission. We have also investigated the single and double beta decay process by producing empirical relations. Finally we presume that the above mentioned works will be guidance to the future experiments.

****

Topological and electrostatic properties of diclofenac molecule as a non-steroidal anti-inflammatory drug: an experimental and theoretical study

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Abstract

Diclofenac is the Non-Steroidal Anti-Inflammatory Drug (NSAIDs), which highly inhibits the lipoxygenase pathways and reduces the formation of leukotriene lipids.In this work, we report on measurements and calculations of the electron density of Diclofenac, obtained from high resolution experimental X-ray diffraction data at 100K and theoretical calculations. The structural investigation confirms that the intermolecular interactions of diclofenac molecule present in the unit cell were found to dimer. The analysis of the molecular electron density (by means of quantum theory of atoms in molecules), the electrostatic potential, the crystal packing and intermolecular interactions (through Hirshfeld surface analysis) enables gaining more insight into the nature of the molecule and its ability to interact with other molecules. Furthermore, the topological properties of the dimer interactions are more stable in the crystal phase and the same carboxyl group is forming strong interactions in the human transthyretin enzyme. The electrostatic potential map shows that the high electronegative regions are appeared around the carboxyl group of the diclofenac molecule in the both crystal and protein environment. This study is complemented by a molecular dynamics simulation of the interaction of diclofenac with transthyretin protein, which enables to test the hypothesis made with the charge density analysis.

Keywords: ExperimentalCharge density, Hirshfeld surface analysis, topological properties, electrostatic interaction, Molecular Dynamics

An Overview on Ion Beams in Material Processing

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Abstract

Ion beams plays a wide role to synthesis and modify the properties of dielectrics, semiconductors, metals, ceramics and biomaterials. The flight of ions may tailor the structure, composition, surface topography, optical activity, magnetic and electrical property and so on. Ion beam mixing (IBM) and Ion implantation (II) are the added advantage in tailoring the material in a controlled manner. Thermally immiscible systems can be made as a compound by ion beam mixing. Doping in semiconductors (with controlled dose and depth to achieve the required extrinsic semiconductors) can be done by low energy ion implantation. This technique has and will rule the semiconductor market now and future. The nature of interaction can be understood as follows; the accelerated ions may losses its energy via elastic and inelastic manner when it interacts a target. Different theories (Columbicexplosion model, Thermal spike model, Visco-elastic model and lateral mass transport) were proposed to explain the phenomena responsible for modifications. In mechanical industry the parameters like wear, friction and corrosion can be precisely altered by ion beam techniques. It may open a wide scope on medical industry, food processing and aircraft manufacturing and so on.

Keynotes: IBM, Semiconductor, medical industry, food processing, aircraft

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Enhancing the EDLC Properties of MnO_2/Graphene Nanostructured electrodes for energy storage applications

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Abstract

Pristine MnO_2 and MnO_2/Graphene nanocomposite has been prepared through a facile hydrothermal method under mild condition, and their structure and electrochemical performance are characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Brunauer-Emmet-Teller (BET), X-ray photoelectron spectroscopy(XPS), Thermogravimetric analysis (TGA). XRD reveals the average diameter of 41-55nm. TEM images show spherical morphology for pure MnO_2 and layered structure for MnO_2/Graphene. Capacitive behavior of the synthesized composite electrodes were evaluated using Cyclic voltammetry (CV), Galvanostatic charge-discharge(GCD) and Electrochemical impedance spectroscopy (EIS) by a three electrode system consisting of carbon glassy electrode as reference electrode, platinum wire as a counter electrode and active material used as working electrode. Aqueous 1M Na_2SO_4 solution was used as electrolyte. At a scan rate of $5mVs^{-1.}$ We have achieved maximum specific capacitance of 518 Fg^{-1} was obtained. Steadiness of MnO_2/Graphene nanocomposite was studied up to 5000 cycles.

Keywords: Hydrothermal, Graphene, Transmission electron microscope, X-ray photoelectron spectroscopy, Supercapacitor

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MS2 ISBN NO:9-789388-413282

A Study on Comparison the efficiency of Solar Panel with using Vegetables and Flowers Dyes

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Abstract

Pristine MnO_2 and MnO_2/Graphene nanocomposite has been prepared through a facile hydrothermal method under mild condition, and their structure and electrochemical performance are characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Brunauer-Emmet-Teller (BET), X-ray photoelectron spectroscopy (XPS), Thermogravimetric analysis (TGA). XRD reveals the average diameter of 41-55nm. TEM images show spherical morphology for pure MnO_2 and layered structure for MnO_2/Graphene. Capacitive behavior of the synthesized composite electrodes were evaluated using Cyclic voltammetry (CV), Galvanostatic charge-discharge(GCD) and Electrochemical impedance spectroscopy (EIS) by a three electrode system consisting of carbon glassy electrode as reference electrode, platinum wire as a counter electrode and active material used as working electrode. Aqueous 1M Na_2SO_4 solution was used as electrolyte. At a scan rate of $5mVs^{-1.}$ We have achieved maximum specific capacitance of 518 Fg^{-1} was obtained. Steadiness of MnO_2/Graphene nanocomposite was studied up to 5000 cycles.

Keywords: Hydrothermal, Graphene, Transmission electron microscope, X-ray photoelectron spectroscopy, Supercapacitor

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Experimental Comparison of Solar Still using Normal Method and Black Paint Coated Method

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Abstract

Two different methods of solar still has been designed to improve thermal performance of the solar still. We have committed to analyze the some of the still parameters. Thermometers were used to measure the temperatures of the two solar stills at different parts of the stills. Based on the input and output energy the two solar stills were compared on their efficiency. Practical comparison was conducted to choose which still was the best in efficiency with the same working environment. These techniques are used to compute the solar still maximum thermal performance at black paint coated still. Tungsten oxide (WO_3) sample was prepared using Sodium tungstate solution after 400° C calcinations by Wet chemical method. The optical absorption analysis of samples was performed in UV–Vis range 400–600 nm. Ultraviolet – Visible spectral analysis was used to find its optical transparency. The optical band gap value of the sample is calculated for tungsten oxide nanoparticle as 2.61 eV which is well with the reported band gap energy value.

Keyword: UV–Vis, Sodium tungstate, Thermometers

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MS4 ISBN NO:9-789388-413282

Green Synthesis and Characterization of MgO nanoparticles using Aloe Vera Extract by Solution Combustion Method

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Abstract

Nanotechnology is the most promising technique which can be exploited in many useful ways. It is also referred to as manipulating materials at nano size. Metal oxide nano particles have a wide range of applications in various fields. These can be fabricated in an environment friendly and non toxic manner by Green Synthesis method using plant or leaf extract. Here it is focused on the green synthesis magnesium oxide (MgO) nano particles by solution combustion method using Aloe vera plant extract as a fuel. The synthesized nano particles were characterized by powdered X-RAY diffraction (XRD), Fourier Transform Infrared (FTIR), Energy Dispersive X-ray Spectroscopy (EDAX) and Ultra Violet (UV) analysis. XRD analysis revealed the formation of cubical structure of MgO nano particles with average particle size of 33nm. EDAX profile confirmed the signal characteristic of Magnesium. The functional groups and compounds responsible for nano particle formation and stabilization were studied by Fourier transform infrared (FT-IR) spectroscopy. The absorption patterns were analyzed by UV-visible spectroscopy.

Keyword: Green Synthesis, Aloe Vera extract, MgO Nano particles

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Green Synthesis and Characterization of Ni doped MgO Nanoparticles by Solution Combustion method using Aloe Vera extract

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Abstract

The green synthesis of metal oxide nano particles through plant extract is simple, eco-friendly, cost effective, and less time consuming. Plant extracts helps in reducing metal ions in the synthesis of nano particles. The present study deals with the green synthesis of Ni doped MgO nano particles by solution combustion method using Aloe Vera plant extract as a fuel. The structural and compositional analyses were done by powder X-ray diffraction (XRD), Energy Dispersive X-ray Spectroscopy (EDAX) respectively. XRD analysis revealed the formation of cubical structure of Ni doped MgO nano particles with average particle size of 31nm. EDAX profile confirmed the signal characteristic of Magnesium and nickel. The functional groups and compounds responsible for nano particle formation and stabilization were studied by Fourier transform infrared (FT-IR) spectroscopy. The absorption patterns were analyzed by UV-visible spectroscopy.

Keyword: Green Synthesis, Aloe Vera extract, Ni doped MgO nanoparticles

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Green Synthesis of Silver Nanoparticles using the Leaf Extract of Kalanchoe Pinnata

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Abstract

The green synthesis of nanoparticles (AgNPs) has more advantages because they are safe to handle and of their easy availability. In this paper, we have described the green synthesis of Silver nanoparticles using the leaf extract of KALANCHOE PINNATA. The synthesized Silver nanoparticles were characterized by x-ray diffraction (XRD), UV-VIS spectrometer, FTIR, SEM with EDAX and PL. kalanchoe species have been used to treat ailments such as infections, rheumatism and inflammation. This method has greater advantage than physical and chemical methods.

Keyword: Silver nitrate, Kalanchoe Pinnata, XRD, UV-Vis, FTIR, SEM

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Synthesis of SnO_2 Nanoparticles by Hydrothermal method and Study of their Properties

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Abstract

In the present work, SnO_2 nanoparticles were synthesized by hydrothermal method and annealed at 400˚C and 800 ˚C in air. Synthesized samples were characterized by powder X-ray diffraction; UV-DRS absorbance spectroscopy and Fourier transform spectroscopy (FTIR) techniques. The crystalline sizes were calculated from X-ray diffraction pattern using Scherrer's formula and it was found that the crystalline size was increased by increasing annealing temperature. Optical bandgap was calculated as 3.4, 3.6 and 3.9 eV as synthesized, annealed at 400˚C and 800 ^{o}C respectively. Surface functional group of synthesized nanoparticles was analyzed by using Fourier transform spectroscopy (FTIR).

Keyword: Optical bandgap, Scherrer's formula, UV-DRS absorbance spectroscopy

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MS8 ISBN NO:9-789388-413282

Preparation and Characterization of Pure and Lithium doped ZnO Nanoparticles

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Abstract

In this present work, the synthesis of pure and Li doped zinc oxide nanoparticles by hydrothermal method using zinc nitrate and sodium hydroxide synthesized and has been reported. CTAB added in nanoparticles preparation, where CTAB used as the size reducing reagent, is one of the most essential properties for the nano particles preparation and its characterization. The synthesized zinc oxide nanoparticles were characterized by X-ray diffraction (XRD), Fourier Transform Infrared (FTIR) Spectroscopy and UV Visible Spectroscopy.

Keyword: Pure and Li doped ZnO NPs, Hydrothermal method, XRD, FTIR, UV-Vis spectroscopy

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Hibiscus rosa sinensis assisted green synthesis of Cadmium oxide nanoparticels

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Abstract

Preparation of metal nanoparticles has been done through the physical and chemical methods. But the new method of green synthesis of nanoparticles through the plant extract is rapidly studied and developed due to the ease in formation of nanoparticles through environment friendly method. This process minimizes harsh and toxic nature of nanoparticles could be reduced. These natural nano factories open up a faster and large scale production of nanoparticles. In this paper Hibiscus flower petals are taken to prepare cdo nanoparticles. X-ray diffraction was accomplished to study the formation of cadmium oxide nanoparticles. UV visible spectrum was carried out to monitor obtained nanoparticles. Also the functional groups present in the prepared nanoparticles were identified. Thus cdo nanoparticles were synthesized inexpensively.

Keyword: Nano-particles, Nano-factories, toxic, Eco-friendly

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MS10 ISBN NO:9-789388-413282

Effect of Sodium Nitrate on the Growth, Optical, Thermal, Nonlinear Optical and Antimicrobial Properties of Γ-Glycine Single Crystal

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Abstract

In this paper, we report the successful growth of sodium nitrate added glycine single crystals by the slow evaporation method. Powder X-ray diffraction analysis confirms the grown γ-glycine crystallizes into a hexagonal structure with a space group of $P3_1/n$. The percentage of transmittance of the crystal was recorded using UV–Vis Spectrophotometer and the optical band gap Eg was estimated for γ-glycine single crystal. Differential scanning calorimetry technique was employed to determine the phase transition, thermal stability and melting point of the grown crystal. The antibacterial activities of the title compound were performed by agar disk diffusion method against the standard bacteria's such as proteus, Staphylococcus aures, Streptococcus aures, Klebsiella and shigella.

Keyword: agar disk diffusion method, Differential scanning calorimetry, γ-glycine single crystal

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MS11 ISBN NO:9-789388-413282

Effect of $MnSO_4$ on the Growth, Optical, Structural, Biological Properties of B-L -Glutamic Acid Crystals

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Abstract

In this paper, we report the successful growth of $MnSO_4$-added β-glutamic acid single crystals by the slow evaporation method. Structural confirmation of the grown polymorph was carried out by powder x-ray diffraction study. UV–Vis-NIR spectral analysis the optical transparency of grown crystals. Differential scanning calorimetry technique was employed to determine the thermal stability and melting point of the grown crystal. The in vitro antimicrobial activity of grown crystals was analyzed against gram positive and gram negative bacteria's carried out by disk diffusion method and found that the crystal shows good inhibition efficiency against various bacteria's strains. DPPH radical scavenging study, exhibit good antioxidant activity and calculated the IC_{50} value of grown crystals, this value comparable with standard Vitamin C. The superior antibacterial activity of L-glutamic acid polymorphs affects against pathogens, having good cell viability against breast cancer cell lines and it can be used in pharmaceutical field for medical applications.

Keyword: UV–Vis-NIR spectral analysis, optical transparency, disk diffusion method

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Synthesis and Characterization of Ni -doped MnO_2 Nanoparticles by Co - Precipitation Technique

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Abstract

The thrust to develop eco - friendly production of nanoparticles arises from the extremely recent nanotechnology research, which gives considerable importance to expand their application. Nickel doped MnO_2 nanoparticles were prepared by co- precipitation method. The Crystalline size of prepared samples was determined by X- ray diffraction. The optical properties of the nanoparticles were analysed using UV-Vis spectroscopy. The surface morphology of the synthesised Ni - doped MnO_2 nanoparticles were analyzed using SEM. MnO_2 nanoparticles thus synthesised have large number of potential applications in the field of pharmaceutical industries, sensors, piezoelectric crystals, fuel cell electrodes and catalysis.

Keyword: X- ray diffraction, UV-Vis spectroscopy, Nickel, MnO_2 nanoparticles

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MS13 ISBN NO:9-789388-413282

Synthesis and Characterization of Fe – doped CdO Nanoparticles by Precipitation Method

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Abstract

In the present study, iron doped CdO nanoparticles were prepared by chemical precipitation method. The synthesized products were characterized by XRD, UV- Vis, SEM. The grain size of cadmium oxide nanoparticles were analysed using XRD.The absorption spectra was recorded in the UV- visible region and analysed. The surface Morphology of the Synthesized nanoparticlesconformed from SEM. Pure CdO reveals ferromagnetic behaviour while antiferromagnetism is observed for all iron doped samples. The synthesized CdO nanoparticles have the great potential application on various industrial and medical field of research.

Keyword: cadmium oxide, SEM, Antiferromagnetism

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MS14 ISBN NO:9-789388-413282

Synthesis and Characterization of Ni doped CdO Nanoparticles by Co Precipitation method

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Abstract

In the present study, the nano structure Ni-doped CdO films have been prepared by chemical precipitation method. The prepared sample were characterized by XRD, UV and SEM .The structural, optical and surface morphology have been confirmed from SEM. The optical band gap values of Ni-doped CdO films were determined by optical absorption method. The particle size of the crystalline determined in Ni-doped of CdO were studied in XRD method. The synthesized CdO nanoparticle has the great studies in various techniques.

Keyword: CdO films, Chemical Precipitation Method

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MS15 ISBN NO:9-789388-413282

Synthesis and characterization of calcium oxide nano particles by Co-precipitation method

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Abstract

Preparation of calcium oxide (CaO) Nano particles is carried out by co-precipitation method. Calciumoxide(CaO) Nano particles is synthesized by using calcium nitrate as a initializing agent and Triethanolamine(TEA) is added which acts as a complexing agent with 0.1M of hydrazine hydrate. The characterization techniques, including XRD and TEM and UVanalysis are taken for the prepared Nano particles.

Keyword: CaO, Tea complexing agent, Co-Precipitation

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MS16 ISBN NO:9-789388-413282

Growth And Characterisation Of Triglycinesulphate (TGS) Single Cyrstal Doped With $NiSO_4$

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Abstract

Synthesis of TGS crystal is done using slow evaporation method.

Glycine is dissolved with Sulphuric acid in distilled water and the solution is doped with $NiSO_4$.Now the required crystal is grown.XRD analysis is done for the grown crystal for structural characterization along with optical analysis.

Keyword: TGS crystal, slow evaporation method, Glycine

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MS17 ISBN NO:9-789388-413282

Classification and Testing of soil types from various places

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Abstract

Soil which is the most important natural resources on earth, is made up of air, water, minerals and organic materials. Soil has an important role in agriculture, filtering and purifying water. Different areas are chosen in Erode district which are Anthiyur, Bhavanisagar, Bungalowpudur, Nambiyur, Kodivery and Koravampalayam.Soil is collected from these places and tested for its fertility. The analysis may be helpful for agriculture, which remains the backbone of our country.

Keyword: Soil, types, Nutrients, Minerals, Resources

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MS18 ISBN NO:9-789388-413282

Synthesis and characterisation of Cupric oxide(CuO) Thin Films by Chemical bath deposition method

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Abstract

Thin films of Cupric Oxide(CuO) are synthesized on the glass slides by chemical bath deposition method. The precursor is prepared by usingCopper Nitrate salt and small amount of Polyvinyl Pyrrolidone and Sodium Hydroxidesolution. Then the glass slides are coated with this precursor by the chemical bath deposition method, which are then analyzed by various techniques like XRD, UVand FTIR.

Keyword: Cupric oxide thin films, chemical bath deposition

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MS19 ISBN NO:9-789388-413282

Effects Of Low Temperature Plasma Treatment On The Bamboo Fabric/Tio_2

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Abstract

This paper investigates the influence of low temperature plasma, on Tio_2 coated with bamboo fabric. Low temperature plasma treatment can modify the surface of Tio_2coated with bamboo fabric and change the substrate characteristics and more importantly, the process is an environmental friendly finishing. The Tio_2 coated with bamboo fabric composites were characterized by several techniques including scanning electron microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR), UV-VIS spectrophotometer, X-Ray Diffraction (XRD) which confirmed the existence of Tio_2 in the composites. The study conclude that was a desirable change in the absorption, transmission, band gap, surface energy and surface morphology.

Keyword: Low temperature plasma, TiO_2, bamboo fabric, substrate characteristics

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MS20 ISBN NO:9-789388-413282

Growth and characterization of Hydantoin-5-acetic acid single crystal

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Abstract

Good quality crystals of Hydantoin-5-acetic acid (HYAA) were grown from aqueous solution at room temperature by slow evaporation method. The crystal structure, spectral, optical and thermal properties have been studied by FTIR, UV-vis spectrum, fluorescence and TGA analyses. The 5-hydantoin acetic acid crystal belongs to the orthorhombic crystallographic system with space group $P2_12_12_1$ [1]. The presence of functional groups in the grown crystal was confirmed by FTIR spectral analysis. The UV-visible spectrum indicates that the crystal is transparent in the entire visible region with a cut-off wavelength of 273.7 nm [2]. The wide optical band gap energy and improved transparency make this crystal suitable for optical devices. TGA study confirmed the thermal stability of the grown crystal.

Keyword: Hydantoin-5-acetic acid, Slow evaporation method, FTIR, UV-Vis spectrum, TGA

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MS21 ISBN NO:9-789388-413282

Synthesis, growth and optical properties of an efficient non linear optical single crystal: 5- chloro 1-methyl -4-nitroimidazolonium salt of malic acid

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Abstract

In this paper, we report the synthesis, growth and characterization of new organic NLO crystal of 5-chloro-1-methyl-4-nitroimidazolonium salt of malic acid (CMNIMA). The title compound is synthesized and crystal was grown by the slow evaporation solution growth technique at constant temperature. The grown crystals have been characterized by power XRD, FT-IR, UV-Vis, Fluorescence, SHG, Dielectric and thermal analysis. The crystalline nature of the grown crystal was confirmed using power X-ray diffraction technique. Presence of various functional groups of the CMNIMA crystal was characterized by Fourier transform infra-red spectrum (FT-IR) and Non -linear optical property is examined by Kurtz powder technique. Hence it may be useful for the Second Harmonic generation (SHG) applications. The optical behavior was analyzed by UV-Vis spectrum and found that the crystal is transparent in the region between the 200-1100nm. The Fluorescence emission spectrum of the title crystal shows violet emission. The Dielectric studies show that the Dielectric constant and Dielectric loss decrease exponentially with frequency at different temperatures. The crystal was thermally stable up to 250°c as determined by DSC-TGA studies.

Keyword: Slow evaporation method, FTIR, UV-vis spectrum; TGA; Second Harmonic generation

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MS22 ISBN NO:9-789388-413282

Synthesis of copper oxide nanoparticles using co- precipitation method

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Abstract

Metal and metal oxide particles are intensively pursued because of their prominence in different field application in science and technology.

In this copper oxide nano particle are synthesized by co-precipitationmethod in which copper nitrate is mixed with polyvinyl pyrrolidone to yield copper oxide nano powder, It is characterized by using XRD, FTIR, and particle analyser.

Keyword: Copper nitrate, polyvinylpyyrolidone, co-precipitation

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Green Synthesis of Cu/HPA-PANI Nanocomposites and Characterization for their Conductivity and Biological Applications

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Abstract

Conducting polymer composites has immense fascinating applications owing to their physical properties. Metal nanoparticles with conductive polymers can result in composite materials having unique physical and chemical properties that can have wide application potential in diverse areas. The present work comprises with the green synthesis of Cu NPs from *Albizia procera* bark extracts. Copper nanoparticles were fabricated in polyaniline (PANI), by *in situ* polymerization method under the action of Heteropolyacid. The synthesized nanocomposites were studied for Optical absorption in the UV-visible region of these suspensions was measured in the range of 200-500 nm and FTIR analysis. Morphology and structure of the composites were characterized by field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD) and Fourier-transform infrared spectra (FTIR). Pure copper nanoparticles were uniformly dispersed into the polymer matrix. Thermal stability of the composites was characterized by thermogravimetric analysis (TGA). Electrical conductivity measurements indicated that the conductivity of the composites was significantly modified than that of pure polyaniline. Also, few *in vitro* antioxidant studies were carried out on these composites through DPPH, H_2O_2, Superoxide radical- scavenging assays, which revealed the biological potential of the composites.

Keyword: Cu NPS, Polyaniline, Thermal Stability, Nanocomposites

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Optical, Cyclic voltammetry and antioxidant studies of Cobalt doped /HPW-PANI Nanocomposites grown by Chemical and Electropolymerisation

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Abstract

Transition metal ion doped Heteropolyacid (HPW)- Poly-chloroaniline (PCA) composites was successfully prepared by *in-situ* oxidative polymerization of aniline monomer for electrochemical application. Cobalt nanoparticles were green synthesized from *Albizia amara* bark extract by precipitation method. The Co NPs were doped with HPW/PCA to synthesize composites which showed improved electrical properties compared to virgin PCA. All the materials were characterized by Fourier transform infrared spectroscopy (FT-IR), UV spectroscopy, field emission scanning electron microscopy (FESEM), XRD studies. The electrochemical capacitive performance of the composites was tested by cyclic voltammetry (CV). The synthesized nanocomposites showed good adherent behavior on electrode surface at pH 1.0, which stamped the presence of oxidation peaks at 0.271 V and 0.623 V and reduction peaks at 0.832 V and 0.493 V. Further, these composites were submitted for antioxidant studies which projected its fine inhibitions through DPPH, H_2O_2, Superoxide radical- scavenging assays.

Keyword: Cobalt nanoparticles, FESEM, cyclic voltammetry

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MS25 ISBN NO:9-789388-413282

Synthesis, Characterization and Application of Nano carbon Composite

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Abstract

Nano Carbon Composite was prepared from the stems of *AlternantheraSessilis*using green procedure. Nano carbon particle (NCP) was prepared from the stems using waste engine oil as precursor, LPG fuel mixed with air and combustion chamber. The Y and Fe co-doped TiO_2photocatalyst was prepared by sol-gel process using ($Ti(OBu)_4$), ethanol, acetic acid, 0.1M $Fe(NO)_3$ and 0.1M $Y(NO)_3.6H_2O$. $Y/Fe/TiO_2$ co-doped nano carbon composite was prepared by stirring 0.5g of NCP using a magnetic stirrer for about half an hour, then transparent sol containing $Y/Fe/TiO_2$ was slowly added with constant stirring. The solid composite was obtained after stirring, drying and calcined for 3 h at a temperature of 450°C under constant flow of N_2 gas. The powdered composite christened as Nano Carbon Sphere (NCS) is used for the photocatalytic degradation of various dyesand the composite catalyst is capable of degrading more dye molecules under visible light.

Keyword: Nano carbon composite, AlternantheraSessilis, Photocatalyst, Visible light

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MS26 ISBN NO:9-789388-413282

Studies on the influence of parameters on photocatalytic activity of polymer nanocomposites- An Overview

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Abstract

Dyes present in the industrial waste water enter the water bodies such as rivers, lakes and pollute the environment. This contaminated water contains highly hazardous and colored pigments which deplete the dissolved oxygen in water and affects the aquatic life and human beings. In order to maintain the quality of the water, several methods were used such as adsorption, electro coagulation, ultrasonic decomposition, etc., to treat the waste water. These conventional techniques were not effective because it leaves the secondary waste which cannot be treated or dumped into the ground due to its carcinogenic nature. Hence an ecofriendly and simple technique called advanced oxidation process (AOP) which uses the hydroxyl radical to degrade the wide range of dyestuff were effective in treating the dye effluents. Among the advanced oxidation process the photo catalysis has been gaining interest from the academic and industries. Inspite of its potential to treat the dye effluents, there are number of factors responsible for the photo catalytic system. These are the parameters govern the photo degradation of the dyes. A number of studies have been reported on the significance of these operational parameters. Some of the factors influence the photo catalysis is the amount of photo catalyst, pH of the solution, temperature of the reaction medium, light irradiation time, the intensity of light, surface area of the photo catalyst, nature of the photo catalyst, dissolved oxygen in the reaction medium, nature of the substrate, doping of metals and non-metals and the structure of the photo catalyst. A number of literatures reported on the operational parameters govern the photo catalytic activity of the polymer nanocomposites. Hence this review is focused on the factors responsible for the effective photo catalytic activity of polymer nanocomposites in the past and also the recent advances in this field for the degradation of dyes.

Keyword: Hazardous, Photo Degradation Photo Catalyst, Adsorption

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MS27 ISBN NO:9-789388-413282

Cost Effective Green Method For The Synthesis Of Silver Nanoparticles

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Abstract

The use of Silver nanoparticles (AgNPs) has been greatly enhanced in biomedical field due to its excellent antimicrobial activity against several pathogenic bacteria. It is used as coatings in dressings, medicinal devices, nanogels in cosmetics and lotions. The physical and chemical synthetic processes involve high temperatures/pressure and the use of hazardous chemicals for the reaction. The recent research involves the synthesis of silver nanoparticles by ecofriendly green methods. Plants flower extract are considered cost-effective and environment friendly for the synthesis of silver nanoparticles. The present study deals with the synthesis of silver nanoparticles using the flower extracts of Aerva Lanata and Gomphrena globosa. The as-formed silver nanoparticles were characterized by UV-Visible spectrophotometer, Fourier Transform Infrared spectroscopy (FTIR), Scanning Electron Microscopy (SEM). The antibacterial activity of the as-synthesized silver nanoparticles was also investigated.

Keywords: Silver Nanoparticles, UV, FTIR, SEM, Antimicrobial activity

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MS28 ISBN NO:9-789388-413282

Degradation of Reactive Yellow Dye Effluent

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Abstract

One of important contaminant that can create health hazard in water bodies is the dye effluents. Many important technologies are currently available for treating wastewater from the textile industry like biological treatment, chemical precipitation, ultrafiltration, carbon adsorption, and oxidation with ozone. But they generally lack the broad scope treatment efficiency required to reduce all the diverse pollutants present in textile wastewater. Electrochemical technology has shown that many of the major chemical components in textile industry wastewater can be effectively and economically removed. The target may be the reduction of COD, requiring the complete oxidation of dyes to carbon dioxide or the removal of colour. In the present study, synthetic dye effluent containing 500 ppm reactive yellow 107 was electrolysed under galvanostatic condition using APLAB model (SPECTRA LAB) wherein the current was controlled with a precision of ± 1%. Electrolyses were carried out using graphite anodes at various pH from 1.0 to 13.0 and NaCl was used as supporting electrolyte. The current density, pH were optimized. To ascertain the removal of dye during electrolysis, UV-VIS were carried out. The dye solution showed absorption at 235 and 387 nm. The first absorption is sharp, arising due to π-π^* absorptions of benzene rings. The second absorption is broad and it may be assigned for the through resonance possible in the molecule. The complete decolourisation of the effluent and the absence of absorption peaks were noticed which suggest complete destruction of the dye and this does not produce any smaller organic units.

Keyword: Electrolysis, Destruction of dye, COD reduction, Effluent treatment, Electrochemical treatment

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MS29 ISBN NO:9-789388-413282

Biosynthesis, Characterization and Antibacterial Studies of Copper Oxide Nanoparticles using Coffee Seed Extracts

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Abstract

The copper oxide nanoparticles (CuO NPs) were synthesized using coffee seed extracts as a reducing agent and copper nitrate as a precursor by adopting eco-friendly method. The synthesized CuO NPs were characterized by X-ray diffraction, UV-visible spectroscopy, Scanning electron microscope, Fourier transform infrared spectroscopy and Particle size analyzer. Further, the antibacterial activity of synthesized CuO NPs was tested against both gram positive and gram negative cultures. Thus, from the above studies, the presence of CuO NPs were confirmed and the synthesized CuO NPs found to exhibit significant antibacterial action which can be employed for various therapeutic applications.

Keyword: CuO NPs, coffee seeds, Fourier transform infrared spectroscopy, X-ray diffraction

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Exploring the Characterization of Copper Oxide Nanoparticles using Eichhornia Crassipes Leaves extract via Bio-Synthesis Method

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Abstract

Bio-synthesis of metal oxide nanoparticles are receiving great attention due to their unique physical and mechanical properties and also gaining promising application in various fields particularly medicine, electric, magnetic field and so on. In this work, copper oxide nanoparticles (CuO) were synthesized using Eichhornia crassipes leaf extract using NaOH by adopting simple, cost effective and eco-friendly method. The synthesized nanomaterials were characterized by Ultraviolet-visible spectroscopy, Antibacterial activity, Fourier transform infrared spectroscopy, X-ray diffraction, Scanning electron microscopeand Particle size analyzer. Thus, the presence of copper oxide nanoparticles has been confirmed from the studies and utilized for various bio-medical activities.

Keyword: Eichhornia crassipes, Fourier transform infrared spectroscopy, Particle Size analyzer, Antibacterial activity

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Conducting properties of new Poly (m-toluidine-co-4-fluoroaniline) nanocomposites with silver nanoparticles

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Abstract

A new series of silver nanoparticles embedded in poly (m-toluidine-co-4-fluoroaniline) copolymer nanocomposites was synthesized by chemical oxidative *in-situ* polymerization method. The characterization of these nanocomposites was carried out by using FTIR, UV-visible spectroscopy, X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM). The synthesized conducting copolymer shows good solubility in common organic solvents such as DMF and DMSO. X-ray diffraction (XRD) pattern reveals the crystalline nature of the copolymer. The scanning electron microscopic study shows the nanotubular sea coral like granular particles that are agglomerated in nature. The increase in conductivity is also due to the interfacial interaction of Ag nanoparticles with poly (m-toluidine-co-4-fluoroaniline) matrix. The electrical conductivity of the compressed pellet of these polymers was measured by the four probe method.

Keyword: m-toluidine, 4-fluoroaniline, DBSA, Ag nanoparticles, conductivity

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Green synthesis of zinc oxide nanoparticles using G*loriosa superba flower* extract and their characterization

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Abstract

Green synthesis of zinc oxide nanoparticles using green plants is a very cost effective, safe, nontoxic, eco-friendly route of synthesis which can be used for the manufacture at a large scale and promising alternative to traditional method of chemical synthesis. In the present work, we report the synthesis of zinc oxide nanoparticles by biological method. The aqueous flower extract of Gloriosa Superba acts as a solvent with manifold roles as promoter, stabilizer and template for the synthesis of nanoparticle. The formed nanoparticles were characterized byX-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR),Scanning Electron Microscopy (SEM), Energy Dispersive X-ray spectroscopy (EDAX) and Ultraviolet visible spectroscopy (UV-vis).*Invitro*antibacterial activity of the synthesised nanoparticles were studied using pathogenic bacteria such as *E.coli*and*StaphylococcusAureaus*. The study was further initiated and reported that Zinc oxide nanoparticle can be used as an inexpensive and effective adsorbent for the removal of arsenic ions from aqueous solution. This approach offers environmentally beneficial alternatives to more hazardous chemicals and processes and promotes pollution prevention by the production of nanoparticle in their natural environs.

Keyword: Nanoparticles, Green synthesis, Zinc acetate, Sodium hydroxide, Gloriosa Superba

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Facile preparation of polymer metal oxide nanocomposites by "mechanical mixing approach"

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Abstract

In the last few decades the development of polymer nanocomposites has been drastically increased because of its wide range of applications in many fields. Polymer nanocomposites have both natural and synthetic types that play an essential role in everyday life. Polymer nanocomposites offer significant development in advanced materials. Here, we use Poly-Ortho-Toluidine (POT) an organic polymer when combined with antimony oxide (Sb_2O_3) an inorganic material, these polymer nanocomposites properties are improved and hence it has lot of applications and have high electrical, thermal and mechanical properties. POT-Sb_2O_3 nanocomposites are prepared by mechanical mixing method. The resultant polymer nanocomposites are characterized by using FTIR, UV-vis, XRD and SEM&EDAX. FTIR is used to investigate the stretching vibrations and functional groups of POT- Sb_2O_3 nanocomposites. The optical properties and interaction between POT and Sb_2O_3 has been studied using UV-visible spectroscopy. XRD analysis proves the prepared sample have high crystalline nature with compared to pure POT. SEM analysis shows the morphology of the sample, the prepared sample have hexagonal structure. EDAX analysis identifies the chemical composition of the sample. The result shows the POT and Sb_2O_3 have strong interaction between them.

Keyword: Poly-Ortho-Toluidine (POT), antimony oxide (Sb_2O_3), nano composites

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PVP – Surfactant – mediated Synthesis & Characterization of WO_3 Nanoparticles

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Abstract

In the present work, Tungsten Oxide (WO_3) powder was synthesized by Wet chemical method in presence of capping agent namely polyvinyl pyrrolidone (PVP). Here, Sodium tungstate dihydrate dissolved in deionised water act as precursor solution. The synthesized powder was characterized by X-ray powder diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR) and UV-visible absorption (UV–Vis) studies. These results showed that the crystallinity, functional groups and the optical property of WO_3 nanoparticles.

Keyword: WO_3, PVP, band gap energy

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Electron transport Performance of CeO_2 Doped TiO_2 nanoparticles in Dye Sensitized Solar Cells

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Abstract

The sol-gel synthesis is promising a new material fabrication method for nanoscale materials and nanotechnology. Mesoporous high surface area and high crystallinity MO2 (M = Ti, Ce, nanopowders were synthesized by a modified sol-gel method using metal alkoxide and acetylacetone. The prepared powders had crystalline size of about 5-10µm, Mesoporous $CeO_2$and CeO_2nanopowders responding to visible wavelength were also obtained by using the same process. A small addition (5 mol %) of CeO2 did not affect anatase phase. However, further addition of CeO_2 increased while anatase TiO_2 decreased. These synthesis methods provide simple route to fabricate nanostructured materials under mild conditions. The synthesized nanoparticles were characterized using X-ray diffraction, field-emission scanning electron microscopy, UV-visible spectrophotometry,Photoluminescence and electrochemical impedance spectroscopy. The results indicated that the adsorption of anthraquinone dyes through the CeO_2 doped TiO_2 was increased along with enhancing the short-circuit photocurrent and open-circuit voltage of the cell. An optimal power conversion efficiency of 3% was obtained in a dye-sensitized solar cell (DSSC) containing the CeO_2doped TiO_2 film. This material combination is a highly promising agent for the enhancement of the conversion efficiency for the fabrication of high efficient, low cost and high stable DSSCs

Keyword: N3 and N719 dye, CeO_2, TiO_2,DSSC .,EIS and SEM

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Study of Geometrical, Electronic Structure, Spectral and NLO Properties of Red Prickly PearSensitizer for Solar Cell Applications

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Abstract

The geometries, electronic structures, polarizabilities, and hyperpolarizabilities of organic dye sensitizer red prickly pearwere studied based on HF and Density Functional Theory (DFT) using the hybrid functional B3LYP. Ultraviolet-Visible (UV-Vis) spectrum was investigated by Time Dependent DFT TD-DFT Features of the electronic absorption spectrum in the visible and near-UV regions were assigned based on TD-DFT calculations. The absorption bands are assigned to $\pi \rightarrow \pi^*$ transitions. Calculated results suggest that the three excited states with the lowest excited energies in red prickly pearis due to photo induced electron transfer processes. The interfacial electron transfer between semiconductor TiO_2 electrode and dye sensitized prickly pear is due to an electron injection process from excited dye to the semiconductor's conduction band. The role of anthroquinonegroup in red prickly peargeometries, electronic structures, and spectral properties were analyzed.

Keyword: DFT, red prickly pear, DSSC, Band Gap

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MS37 ISBN NO:9-789388-413282

Synthesisand Characterization Of Poly(Aniline-O-Toluidine) Copper Oxide Nanocomposites For Biomedical Applications

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Abstract

Synthesized P(ANI-OT) CuOnanocomposites is used to polyaniline, poly-o-toluidine, CuO by emulsion polymerization method. In this method potassium dichromate as an oxidant in aqueous sulfuric acid under constantstirring at 60°C in presence of Nitrogen gas atmosphere.The different weight percentages of CuO (25%, 50% and 75%) are added during the polymerization.The synthesized composite were characterized byvarious analytical techniques such as, FTIR, XRD, UV, SEMand EDAX. Also the antibacterial activity analyses are carried out.Thefunctional groups are conformed by FTIR analysis. The XRD pattern is nature of the composite and UV-Vis analysis is the find the optical properties and band gap energy. Surface morphology is studied using Scanning Electron Microscopy (SEM) with EDAX analysis is confirmed by the chemical composition of composite. Antibacterial activity analysis is the good resistivity towards the bacterial growth.

Keyword: Poly(aniline-O-Toluidine), CuO Nanocomposites, SEM, Antibacterial activity.

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X – Ray Diffraction Study of Tungsten oxide Nanoparticles synthesized by Wet Chemical Technique

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Abstract

Tungsten oxide (WO_3) sample was prepared by Wet chemical method using sodium tungstate solution as precursor. Nanocrystalline WO_3 powder was obtained after 400° C calcinations. The physical property of the synthesized Tungsten oxide material was characterized by X-Ray Diffraction. The predominant peaks obtained in X-ray diffraction pattern reveal the crystalline nature of the sample and the structure belongs to Monoclinic WO_3. XRD assessed result indicates the crystalline improvement along (020) orientation and maximum crystallite size of the plane (020) was found to be 32 nm.

Keyword: XRD, monoclinic crystalline

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MS39 ISBN NO:9-789388-413282

Synthesis and Structural morphology with Antibacterial activity of Zn/Ag capped Hydroxyapatite by Wet Precipitation Method

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Abstract

Due to effective biocompatibility and bioactivity of Hydroxyapatite, it plays an essential role in medicinal field in particular as bone substitute and coating for implants. The main aim of this study is to incorporate two divalent cations (Silver and Zinc) in HAp as capping agents by wet precipitation method. FTIR, XRD, EDAX and SEM are used for its characterization to analyze functional group, phase composition, crystalline size, elemental composition and the surface morphology. The antibacterial activity of the synthesized nanoparticles is tested against two gram positive and two gram negative bacteria.

Keyword: Hap, biocompatibility, FTIR, XRD, EDAX

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Synthesis and Characterization of Ti/Ag capped Hydroxyapatite by Sol-Gel method

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Abstract

HAp is effectively used as bio implant material because it closely resembles bone apatite and exhibits good bio-compatibility. This paper explains the synthesis of Ti/Ag capped HAp by sol-gel method. The HAp nanoparticles were characterized by XRD to study the crystalline size and Phase composition, SEM for surface morphology, FTIR for Functional group and EDAX for elemental composition. The antibacterial activity of the synthesized (Ti/Ag) capped hydroxyapatite was studied against both two gram positive and two gram negative bacteria.

Keywords: HAp, Bio-compatibility, FTIR, XRD, SEM

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MS41 ISBN NO:9-789388-413282

Synthesis And Characterization Of Polypyrrole-Zinc Oxide Core-Shell Hybrid Polymer Nanocomposites

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Abstract

Synthesis of hybrid functional nanocomposites (PPy-ZnO) was employed with ZnO by mechanical mixing method, this system, the observed FT-IR result ensured the presence of PPy in the composite and also pronounces the characteristic absorption peaks of ZnO around 591 and 438 cm^{-1}. The observed strong vibration in the low wave number region around 591cm^{-1} is corresponds to antisymmetric vibrations of Zn-O-Zn bond of Zinc oxide. This ensured the presence of ZnO incorporated in the PPy nanoparticles. UV-Vis absorption spectra of PPy-ZnO nanocomposites helps to explore the optical behavior of incorporated nanoparticles into PPy matrix and hence, the integrated ZnO nanoparticles gives rise to the red shift of π–π* transition of polypyrrole. SEM images reveal that ZnO nanoparticles is deposited on the PPy surface which have a nucleus effect on the polymerization of PPy. It also ensures, the degree of deposition on the surface of PPy increases with ZnO content. SEM images indicated that the zinc particles are embedded in the PPy matrix forming the core-shell structure. ZnO nanoparticles exist as agglomerates due to high surface area and magneto dipole-dipole interactions between the particles. In SEM images, the black core is zinc particles with the diameter range of 50-150 nm and the light colored shell is attributed to PPy in the nanocomposites, which is due to the different electron penetrability. The EDAX results of PPy-ZnO reveals that an elements like Carbon (44.23 wt.%) and Sulfur (3.18 wt.%) molecules decreases and Zinc (23.47 wt.%), Oxygen(29.12 wt.%) molecules increases, while increasing concentration of ZnO nano metal oxide content.

Keyword: PPy-ZnO, EDAX, π–π* transition, SEM

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MS42 ISBN NO:9-789388-413282

Preparation and characterization of novel hybrid organic-inorganic (Poly-O-Toluidine-CdO) polymer nanocomposites

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Abstract

An organic-inorganic hybrid Poly-o-toluidine-CdO (POT-CdO) nanocomposite has been synthesized by Insitu chemical oxidative polymerization method. The prepared pure POT and POT-CdO (50%) polymer nanocomposite are characterized by using FTIR, UV-Vis, XRD, SEM, EDAX and antimicrobial activities. In FTIR spectra reveals the information of functional groups (N-H, C-H, C-C, C=C) in pure POT and POT-CdO (50%) nanocomposites also confirm interaction between POT and CdO nanoparticle, The optical absorbance of pure POT and POT-CdO was measured in the range of 250-1000 nm. This absorption spectrum shows two absorption bands centered at 316, 622 nm (pure POT) and the optical band gap energy is (3.93 eV, 1.99 eV) and 314, 613 nm are observed in POT-CdO (50%) nanocomposite and the optical band gap energy is (3.95 eV, 2.02 eV). The XRD pattern of pure POT shows the amorphous nature and the XRD pattern of POT-CdO nanocomposites reveals high crystalline material. The SEM micrograph of POT has porous and irregular structure and POT-CdO nanocomposites are highly agglomerated and form cluster spherical shaped morphology due to Vander Waals force of attraction, the morphology of the material has been confirmed with the formation of organic-inorganic nanocomposite material. The EDAX spectrum of pure POT and POT-CdO nanocomposites C, S, O and Cd elements are present in different weight percentage. The antibacterial activity of pure POT and POT-CdO nanocomposites against gram positive and gram negative were observed using agar well diffusion method. It was also found that POT-CdO has enhanced antibacterial activity compared to pure POT.

Keyword: Poly-O-toluidine (POT), Cadmium oxide (CdO), Nanocomposites, Antibacterial activity

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MS43 ISBN NO:9-789388-413282

Structural, Morphological and Optical properties of Sn doped ZnO thin films

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Abstract

Pure and Sn doped Zinc Oxide thin films were prepared by using chemical bath deposition process. Structural, Morphological and optical properties of the samples were characterized by using XRD, SEM and UV-Visible studies. XRD result showed that decrease in grain size from pure sample due to the incorporation of Sn ions. Bandgap energy values calculated from UV-Visible studies showed that these samples were suitable for optoelectronic applications.

Keyword: ZnO thin film, CBD, XRD, SEM

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MS44 ISBN NO:9-789388-413282

Synthesis Characterization And Anti Bacterial Investigation Of Pure Zinc Oxide And Copper Doped Zinc Oxide

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Abstract

Undoped and Copper doped Zinc Oxide nanoparticles (NPs) have been successfully synthesised by chemical precipitation method. The synthesized NPs have been characterized by number of techniques such as X-Ray diffraction (XRD), Scanning Electron Microscopy (SEM) and EDAX. The antibacterial investigation was done for undoped and Copper doped Zinc Oxide. The XRD analysis reveals that the synthesised samples were crystalline in nature with hexagonal wurzite structure. The grain size decreases with the addition dopants. EDAX spectrum confirms the presence of elemental particles such as Cu, Zn and O. The antibacterial investigation shows that the Copper doped Zinc oxide exhibits greater zone of inhibition than pure Zinc oxide nanoparticles.

Keyword: ZnO nanoparticles, XRD, SEM, EDAX

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Green Synthesis Of Chromium Oxide Nanoparticles By Cucurbita Maxima Extract And Their Antibacterial Activities

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Abstract

Chromium Oxide nanoparticles have been synthesized using Potassium dichromate as a precursor and Cucurbita maxima leaves as a reducing agent by adopting green synthesis method. The synthesized samples were characterized by FTIR, UV-Vis spectroscopy, X-ray diffraction (XRD), Scanning electron microscopy (SEM) and Antibacterial activity. The particle size of the obtained sample has been calculated by Debye-Scherrer formula and calculated value is 8.065 nm. Thus, Chromium Oxide nanoparticles which shows greater effect for fungal culture and utilized for stroppingknives, glasses, inks, paints and precursor to themagnetic pigment. Further, UV-Visible absorption and IR Spectroscopy confirms the formation of nanosized Cr_2O_3.

Keyword: Chromium Oxide, Debye-Scherrer formula, SEM, UV-Vis Spectroscopy

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Theoretical studies on structural properties of dehydroxyascorbic acid and 5-1RD4T

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Abstract

Ascorbic acid (vitamin C) is used to prevent or treat low levels of vitamin C in people who do not get enough of the vitamin from their diets. Most people who eat a normal diet do not need extra ascorbic acid. Low levels of vitamin C can result in a condition called scurvy. Scurvy may cause symptoms such as rash, muscle weakness, joint pain, tiredness, or tooth loss. Vitamin C plays an important role in the body. It is needed to maintain the health of skin, cartilage, teeth, bone, and blood vessels. It is also used to protect your body's cells from damage. It is known as an antioxidant. In the present investigation structural parameters and binding energies of well known antioxidant dehydroxyascorbic acid(DHA) is compared with its similar structural conformer 51RD4T. Density functional theory, a useful concept derived from quantum mechanics mainly focuses over the electronic density around the molecules is used in the present investigation. The geometry of the two vegetable acids are been optimized with the help of Beckes three parameters along with the functions of Lee-Yang and Parr using the triple zeta valence basis set 6-311G(d,p). Thermochemical calculations (frequency) is carried out under room temperature with 1 atmospheric pressure. In order to understand the occupied orbital levels frontier molecular orbital analysis(FMO) is done and corresponding energy gap E gap between the energy levels is found to be 3.23eV for DHA acid and 3.25eV for 51RD4T. Electron donating capability and accepting capability of two flavonoids are been investigated with the help of molecul ar electrostatic potential (MEP).

Keyword: Density functional theory, Vitamin C, molecular properties

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Theoretical studies on electron localization and structural parameters of dexpanthanol and pantothenic acid

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Abstract

Organic acids are one of the major phytochemicals in vegetables and responsible for food taste and odor. Different organic acids are analyzed in fruits and cereals, but least in vegetables and spices. Organic acids has been analyzed because of their high importance in the formation of other phytochemical and increased antioxidant activity. The aim of the present study is to investigate the structural parameters(geometry, ground state energy, electron donating and accepting capability, electronegativity etc.,). Density functional theory – a useful concept derived from quantum mechanics mainly focuses over the electronic density around the molecules is used in the present investigation. The geometry of the two vegetable acids are been optimized with the help of Beckes three parameters along with the functions of Lee-Yang and Parr using the triple zeta valence basis set 6-311G(d,p). Thermochemical calculations (frequency) is carried out under room temperature with 1 atmospheric pressure. In order to understand the occupied orbital levels frontier molecular orbital analysis(FMO) is done and corresponding energy gap (E_{gap}) between the energy levels is found. Electron donating capability and accepting capability of two flavonoids are been investigated with the help of molecular electrostatic potential (MEP). Based on the electron localization function visualization it is observed that the investigated smiliar parental conformations dexpanthanol and pantothenic acid are well stabilized and are capable of donating electron(good behavior to be an antioxidant) rather than accepting electron.

Keyword: Organic acids, Density functional theory, Molecular properties

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MS48 ISBN NO:9-789388-413282

Antibacterial effect of Ag doped ZnO nanoparicles by Sol-gel method

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Abstract

Silver-doped Zinc oxide nanoparticles were synthesized by Sol-gel method. The synthesized Ag -ZnO nanoparticles were analyzed by XRD, FTIR, SEM and Antibacterial activity. The X-ray diffraction pattern clearly showed that the hexagonal wurtzite structure and crystalline Ag-ZnO particles. The crystalline size is in 15 to 31nm. The Fourier Transform Infrared gives the molecular band present in the sample. The Scanning Electron Microscopy images showed that the presence of spherical nanoparticles. The Antibacterial activity of silver doped ZnO nanoparticles were studied using agar well diffusion method.

Keyword: SEM, XRD, FTIR, Antibacterial activity

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MS49 ISBN NO:9-789388-413282

Synthesis and characterization with antibacterial activity of Cu-doped ZnO Nanoparticles by Co-Precipitation Method

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Abstract

ZnO nanoparticles plays a dominant role in medicinal and industrial applications whereas it contains high antibacterial activities. In this synthesis, Cu-doped ZnO nanoparticles are prepared through chemical-precipitation method by using nitrates of metallic precursors. The synthesized samples were characterized by Fourier Transform Infrared Spectroscopy(FTIR), X-Ray Diffraction(XRD), Scanning Electron Microscope(SEM) and Antibacterial activity. The presence of functional groups and chemical bonding are revealed by FTIR spectrum. In X-Ray Diffraction the sharp peaks reveals that the nanoparticles has a different microstructure whereas the hexagonal wurtzite structure will not be changed. The rod-like structure is obtained in SEM micrographs reveals that the substitution of Cu^{2+} ions into the ZnO lattice. In antibacterial activity the synthesized nanoparticles were tested for gram positive and gram negative micro-organisms by using well diffusion method.

Keyword: Crystalline structure, Morphology, Functional group, Antibacterial activity

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MS50 ISBN NO:9-789388-413282

Nano crystalline structure of Magnesium dioxide (MgO_2) using Sol–gel method

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Abstract

Optical property of Magnesium dioxide (MgO_2) by using sol-gel method. Magnesium dioxide (MgO_2) is odourless, fine dioxide which releases oxygen when reacts with water. Magnesium acetate and oxalic acid have been dissolved in ethanol and formed a Magnesium malonate before calcinated at 600˚c for 2 hr to produce Magnesium dioxide (MgO_2) nanoparticles. The crystal structure, morphology, constituent element and optical property of the products using this method were investigated by X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared (FTIR) and Ultraviolet- visible spectroscopy (UV- vis). In our study, we can conclude that the morphology, crystalline size, band gap and molecular structure of particles.

Keyword: Crystalline structure, Morphology, Molecular structure, band gap

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Sol-gel synthesis and characterization of Cu doped TiO_2 nanoparticles with enhanced optical and Structural properties

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Abstract

The pure TiO_2 and Cu doped TiO_2 Nanoparticles at different mole ratios (1%, 2% and 5%) were prepared by using sol-gel method. The prepared nanoparticles were calcinated at 450°C for 2 hours and the nanoparticles were characterized by X-Ray Diffraction (XRD), Field Emission Scanning electron microscopy (FESEM), Energy Dispersive X-Ray Spectroscopy (EDX), UV-Visible spectroscopy (UV-Vis). XRD analysis confirms the formation of anatase titanium dioxide Nanoparticles and the crystalline sizes were increases with increasing the Cu content. FESEM images revealed that the spherical shape with slight agglomeration. EDX analysis confirms the presence of Cu, Ti, O elements. UV-VIS analysis revealed band gap energy of pure and Cu doped TiO_2 Nanoparticles were 2.63, 1.99, 1.88 and 1.45 eV, which improves the photoactive process in the material.

Keyword: TiO_2, Cu doped TiO_2, Nanoparticles, Sol-gel method.

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Role Of Metal-Ions in Wild-Type like and Metal-Binding region mutants of Cu-Zn Superoxide Dismutase 1

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Abstract

About half of all known proteins at present are found to contain metal as one of the cofactors. The interaction studies of metal ions with amino acid help to understand the biological process. The gene corresponding to Cu-Zn SOD1 protein leads to familial form of amyotrophic lateral sclerosis [ALS] due to dominant mutations in the above protein. The mutations in the metal binding region play an important role in ALS pathology, by affecting the protein stability and catalytic activity. The metal-binding region in native state of SOD1 protein and wild-type like mutants and metal-binding region mutants of the same protein are selected to understand the role of divalent metal cations in maintaining the stability and activity of the protein through its interaction with their respective coordinating residues. In the present work, our aim is to examine the strength of cation-π interaction of the above systems by performing quantum chemical calculations using density functional theory. The interaction energies, metal-ion affinity, polarization and dipole moment for the metal-ion binding region in native and mutated states of SOD1 protein have been calculated. The topological properties of the intermolecular hydrogen bond formed between the first and second co-ordination sphere residues leading to interaction of second co-ordination residues with the divalent metal cations in native and mutated states of SOD1 protein have been studied. The NMR chemical shift and spin-spin coupling constants of the intermolecular hydrogen bond were also calculated for native and mutated SOD1 protein.

Keyword: Cu-Zn superoxide dismutase, cation-π interaction, wild-type like mutants, metal-binding region mutants, NMR, spin-spin coupling constants, split valence basis set

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Effect of kinetic energy over structural properties of pectin and quinnic acid– A DFT study

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Abstract

Fruits and vegetables are universally promoted as healthy. The Dietary Guidelines for Americans 2010 recommend you make one- half of your plate fruits and vegetables. Myplate.gov also supports that one-half the plate should be fruits and vegetables. Fruits and vegetables include a diverse group of plant foods that vary greatly in content of energy and nutrients. Additionally, fruits and vegetables supply dietary fiber, and fiber intake is linked to lower incidence of cardiovascular disease and obesity. Fruits and vegetables also supply vitamins and minerals to the diet and are sources of phytochemicals that function as antioxidants, phytoestrogens, and antiinflammatory agents and through other protective mechanisms. In the present investigation pectin and quinnic acid two well known vegetable acids are been investigated for structural properties of kinetic energy distribution. Density functional theory – a useful concept derived from quantum mechanics mainly focuses over the electronic density around the molecules is used in the present investigation. The geometry of the two vegetable acids are been optimized with the help of Beckes three parameters along with the functions of Lee-Yang and Parr using the triple zeta valence basis set 6-311G(d,p). Thermochemical calculations (frequency) is carried out under room temperature with 1 atmospheric pressure. In order to understand the occupied orbital levels frontier molecular orbital analysis(FMO) is done and corresponding energy gap E_{gap} between the energy levels is found. Electron donating capability and accepting capability of two flavonoids are been investigated with the help of molecular electrostatic potential (MEP). Based on the kinetic energy distribution it is evident that the observed results are in line with the observations made for MEP, FMO and molecular descriptor analysis where hydroxyl and carboxyl units posses much electronic movement and are highly unstable making them to easily donate electron.

Keyword: MEP, FMO, Thermochemical calculations

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Preparation Of Polyaniline Zirconium Dioxide (Pani-Zro_2) Nanocomposite Material By In-Situ Method

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Abstract

"In-situ" deposition technique has been employed for the synthesis of conducting pure aniline(PANI) and polyaniline zirconiumdioxide (PANI/ZrO_2) composites in various concentration of(25% and 50%) in the presence of sulphuric acid(H_2S0_4)as dopant by adding fine grade powder of ZrO_2 in polymerization reaction mixture of aniline. Since PANI is the most stable conducting polymer , it is used in the industry along with thermoplastic. The composites obtained were characteristics by FTIR spectroscopy and particle size analyser. The presence of functional groups (C-C,C-H,N-H) has been studied by Fourier transformer infrared spectroscopy.The particle size analyser is used to find the mean size of the particle.

Keyword: In-situ, FTIR, Partical size analyser

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Investigating the interaction of metal cations with dna base-pairs – A Quantum chemical approach

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Abstract

The interaction between nucleic acids and metal cations is the most promising topic at scientific and technological implications. TheMetal cations are found to interact at the various sites of nucleic acids. The interaction of metal-cations with nucleic acids results in significant changes in the stability and the electronic properties of nucleic acids. Herethe interaction of DNA base pairs Adenine-Thymine and Guanine-Cytosine (A-T &G-C) with the metal cations (Na^{2+}, Cu^{2+}, $Mg2^{+}$, Zn^{2+}) were investigated using quantum chemical method. The interaction energy for the base pair and metal cation complexes were obtained. The electron density and molecular bonding pattern of individual electrons and electron pairs were investigated using Natural Bond Orbital (NBO) method. The charge transformation between DNA base pairs and metal cations were studied using HOMO-LOMO calculations.The disturbance of electron density in base pairs after interacting with the metal-cations is obtained from polarization analysis.

Keyword: DNA, base pairs, quantum chemistry, DFT, NBO

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A Quantum Chemical Study On The Interaction Of Aliphatic Amino Acids With Metal Cation

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Abstract

Amino acids are the basic unit of protein. All proteins are enzymes but all enzymes are not protein. Binding of inorganic element especially metal-ions is one of the major functions of protein. In this work the quantum chemical method have been applied to study the interaction of aliphatic amino acids Alanine, Proline, Leusine, Isoleusine and Valine and metal ions ($Ni^{2+,}$ Mn^{2+}, Fe^{2+}). The minimum energy of amino acids before and after interaction with metal ions was predicted. The interaction energy has been calculated for the aliphatic amino acids with different metal-ions. HOMO-LUMO calculation has been performed to explain the charge transfer interactions within the amino acid metal-ion complexes. We carried out NBO analysis, to study the hyper-conjugative interaction and electron density transfer. Polarizability of the amino-acid metal-ion complexes was calculated to study the electronic properties.

(a) (b)

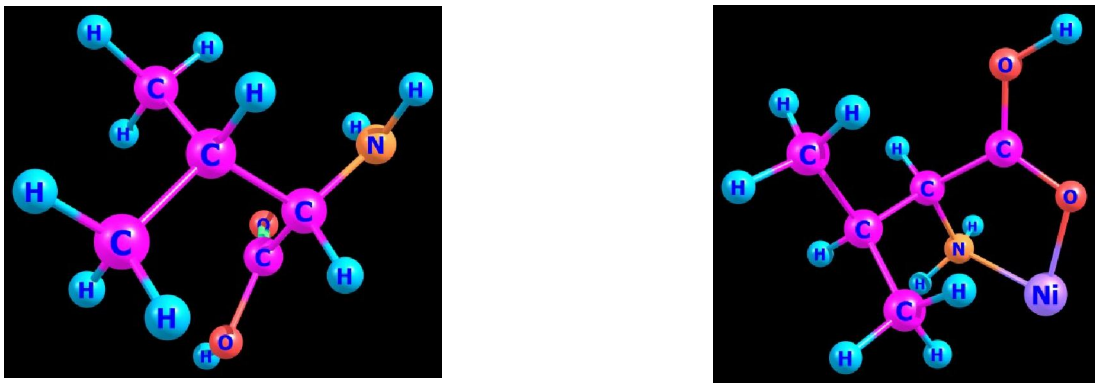

Fig (a) represents the optimized geometry of Vanline before interaction. Fig (b) represents the optimized geometry of Valine after interacting with Nickel cation (Ni^{2+}).

Keyword: amino acid, aliphatic, quantum chemistry, DFT, NBO

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MS57 ISBN NO:9-789388-413282

Synthesis and Characterisation of Zno, CuO and their Composites by Precipitation Method

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Abstract

ZnO, CuO nanoparticles and their composites were prepared by precipitation method. Nano metaloxides have wide range of application in many fields like electronics, fuel cells, batteries, agriculture, medicines etc. The nano powders thus prepared were characterized by UV-Visible spectroscopy, FTIR, XRD, PL, SEM and EDX techniques. UV-visible spectroscopy and PL were carried out for the optical characterization of nano particles. XRD study reveals that the synthesized ZnO, CuO and their composites were crystalline in nature with the average crystalline size range between 32-34 nm. The surface morphology of ZnO exhibits hexagonal shape, CuO exhibits sphere shape with surface porous flower shape and ZnO – CuO composites exhibits flake shape. FTIR confirms the presence of functional groups present in the synthesized samples.

Keyword: SEM, UV-visible, FTIR, XRD, PL, EDX

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MS58 ISBN NO:9-789388-413282

Green Synthesis Of Magnesium Oxide Nanoparticle using Orange Peel Extract

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Abstract

Synthesis of magnesium oxide (Mgo) was employed with orange peel extract due to its very good bio reductant property by green synthesis method. The Mgo particle is helpful to remove the effluent from textile and dying industries. Since the orange fruit contain citric acid, the Mgo act as a reducing agent also it act as antioxidant property. The prepared magnesium oxide was characterized by fourier transform infrared spectroscopy (FTIR), X-Ray diffraction (XRD), scanning electron microscopy(SEM), and antibacterial activity. The functional group has been analyzed using FTIR. The morphological study was confirmed using SEM. The pure monoclinic crystalline structure was resulted from XRD. Also the antibacterial activity was performed against set gram positive and gram negative bacteria.

Keyword: Magnesium oxide, orange peel, FTIR, SEM, XRD, Antibacterial

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Synthesis, Characterization and Antimicrobial studies of Nickel Oxide Nanoparticles by Co-Precipitation Method

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Abstract

Synthesis of metal oxide nanoparticles are focussed on great attention because of their prominence in different field of application in science and technology. In this work, Nickel oxide nanoparticles (NiO) were synthesized by Co-Precipitation Method using Nickel (II) Chloride Hexahydrate (NiCl2.6H2O) and sodium hydroxide (NaOH) as starting material. The synthesized nanomaterials were characterized by Ultraviolet-visible spectroscopy, Antimicrobial activity, Fourier transform infrared spectroscopy, X-ray diffraction, Scanning electron microscope. Thus, the presence of Nickel oxide nanoparticles has been confirmed from the studies and utilized for various potential applications in the field of pharmaceutical industries, sensors, piezoelectric crystals, fuel cell electrodes and catalysis.

Keyword: Nickel Oxide Nanoparticles, UV, FTIR, SEM, Antimicrobial activity

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Preparation Of Polyaniline Nibonium Pentoxide(Pani- Nb_2o_5) Nanocomposite Material by In-Situ Method

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Abstract

The Pure Polyaniline (PURE-PANI) and the PolyanilineNiboniumPentoxide(PANI-Nb_2O_5) at various weight concentration of 25% and 50% has been employed by the "In-situ" method in the presence of sulphuric acid as the dopant.PURE-PANI is highly used in the industry due to their stable conducting property.Thenanocomposite material was resulted and characterised by Fourier Transformer Infrared Spectroscopy(FTIR) and particle size analyser.The presence of functional group (C-H,C-C,N-H,C-N)was examined by the FTIR. The particle size analyser is used to find the mean size of the nanocomposite.

Keyword: FTIR , Particle size analyser, In-situ method

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Effect Of Surfactant On Cadmium Sulfidenanoparticles Prepaed By Precipitation Method

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Abstract

Semiconductor nanoparticle and their synthesis have attracted more in the research field more than hundreds of years because of their optical properties.Cadmium sulfide (CdS) nanoparticle is widely used semiconductor because of its wide band gap energy.In the present study, the effect of surfactant on the structural, surface morphological, optical and photocatalytic activity were analyzed. Cds nanoparticles and anionic surfactant SDS (sodium dodecyl sulphate) assisted CdS nanoparticles were synthesized by chemical precipitation method using cadmium chloride (cdcl2), sodiumsulfide (Na2s), SDSand water as a solvent by fixed temperature 80 degree Celsius.The synthesized nanoparticles were characterized by X-Ray Diffraction, Scanning Electron Microscopy, and Fourier Transform Infrared Spectroscopy, UV-Visible Spectroscopy.

Keyword: Chemical precipitation, SDS, Nanoparticles, XRD, Optical property, SEM

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Activated carbon prepared from tea waste via chemical activation method

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Abstract

In the recent field of research, the researchers have great interest in preparing activated carbon from different organic precursor materials. In the present work, activated carbon sample was prepared from waste cooked tea. Among many organic materials such as turmeric waste, coconut shell, corn cob, rice husk, waste cooked tea is cheap and easily available. TheActivation process was done using dilute sulphuric acid as activating agent.Activated carbon most widely used,because they have large absorptive capacity. The structural and surface morphological of the synthesised sample were analysed using different spectroscopic techniques. XRD, FTIR and SEM were used to characterize the activated carbon prepared from the waste cooked tea. Activating agent with their spectroscopic results suggested that the prepared activated carbon representing an economically promising material with wide spectrum of applications. The important factors affecting the Activated carbon production, the possible applications of Activated Carbon and their future prospects were also discussed.**Keywords**: Waste tea, Sulphuric acid, Activated Carbon, SEM.

Keyword: Waste tea, Sulphuric acid, Activated Carbon, SEM.

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Biosynthesis, Characterization And Antibacterial Studies Of Copper Nanoparticles Using Eclipta Prostrata Leaves Extracts

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Abstract

The thrust to develop eco-friendly production of nanoparticles arises from the extremely recent nanotechnology research, which gives considerable importance to expand their application. The copper nanoparticles (CuNPs) were synthesized using Eclipta Prostrata Leaves extracts as a reducing agent and copper acetate as a precursor by adopting green options method. The synthesized Cu NPs were characterized by X-ray diffraction, UV-visible spectroscopy, Scanning electron microscope, Fourier transform infrared spectroscopy. Further, the antibacterial activity of synthesized CuNPs were tested against both gram positive and gram negative cultures. Thus, from the above studies, the presence of CuNPs were confirmed and the synthesized Cu NPs found to exhibit significant antibacterial action which can be employed for various therapeutic applications.

Keyword: Cu NPs, Eclipta Prostrata, Fourier transform infrared spectroscopy, X-ray diffraction.

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Synthesis and characterisation of surfactant (SDS) assisted cadmium oxide nanoparticles via co- precipitation method

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Abstract

In recent years, nanomaterials have received a great attention due to its physical and chemical properties. Now a days, many attempts to control the shape and size of nanoparticles. Surfactant assisted Cadmium Oxide nanoparticles were prepared by co- precipitation method using cadmium acetate, SDS (sodium dodecyl sulphate) as surfactant, ammonia solution and deionised water (solvent) and the prepared samples were used to maintain the pH value as 8. The Crystallite size of the surfactant (SDS) assisted CdO nanoparticles were calculated using X-ray diffraction (XRD), and the presence of functional groups were analysed by Fourier transform infrared spectroscopy (FTIR). The morphology of surfactant assisted CdO nanoparticles were shown in scanning electron microscopy (SEM) image and the optical band gap was determined by Ultra-violet visible spectroscopy (UV). Thus, the surfactant assisted CdO nanoparticles have various applications in pharmaceutical and food products as well as industrial and commercial cleaning.

Keyword: CdO , surfactant SDS(Sodium dodecyl sulphate), XRD,FTIR,SEM, UV.

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Synthesis And Characterization Of Mg Doped TiO_2 nanoparticles by Sol -Gel Method

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Abstract

Magnesium doped titanium dioxide (Mg- TiO_2) Nanoparticles has been synthesized by sol-gel method and characterized by Fourier Transform Infrared Spectroscopy (FTIR), UV-Visible spectroscopy and Particle size analyzer. FT-IR spectral study along with Mg doped TiO_2 nanoparticles different vibrational modes is calculated. UV-Visible spectroscopy reveals the absorption edge of Mg doped TiO_2 nanoparticles blue shifed longer wavelength and optical band gap was calculated by using Tauc plot for pure TiO_2 (E_g = 3.2 eV) and Mg-doped TiO_2 nanoparticles is lower.Particle size analyzer is used to measure the particle size median values from pure TiO_2, 1% and 0.5% Mg doped TiO_2 nanoparticles are 3.06µm, 0.047µm, and 32.2µm.

Keyword: Magnesium, Titania, sol-gel method, FTIR, UV-Visible and Particle size analyzer.

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Structural and Optical Properties of 4-(6-Methyl-4-phenyl-2-quinazolinyl)-1-pentylpiperazin-1-ium dyes

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Abstract

The experimental and theoretical study on the molecular structure and the vibrational analysis of carbocyanine dye is presented. The FT-IR and FT-Raman spectra were recorded in gas state. Optimized geometry, vibrational frequencies and thermodynamic properties of the title compound were calculated using DFT methods and in good agreement with experimental values. The detailed interpretation of FT-IR and FT-Raman spectra of the compound were reported. The HOM0-LUMO analysis was used to determine the charge transfer within the molecule. In addition to these Mullikan's atomic charges were also reported. Mullikan's atomic charges show charge stability relations. The Electronic transitions measured experimentally by UV-Visible spectrum. According to DTA analysis the substance shows an exothermic peak at 384°C. The Natural Bond Orbital analysis has been carried out in order to study the intra-molecular interaction among the bonds.

Keyword: Mullikan's atomic charge, HOMO-LUMO, Vibrational analysis, Carbocyanine dye, NBO analysis

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DFT and Experimental studies of natual dyes extracted from medicinal plants O*cimum tenuiflorum* and P*iper nigrum* for dye sensitized solar cell applications

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Abstract

The steady increase in 5% global energy requirement per year has necessitated the exploration of alternative sources of renewable energy, which has become a top challenge. The photovoltaic technology has become the most promising technology in terms of harvesting solar energy and converting the same into electrical energy. Due to the limitations of toxicity and high cost possessed by the single crystalline silicon solar cells, the use of dye sensitized solar cells (DSSCs) has gained immense attention towards solar energy harvesting. In particular, the use of natural dyes has become a viable alternative to expensive and precious Ruthenium dyes because of their low-cost, easy attainability, abundance in supply of raw materials and eco-friendly. In this paper, we investigate the performance of DSSCs based on natural dyes extracted from selected Indian medicinal plants. Herein, cubebin and betalain pigments are extracted from fresh *Ocimum tenuifloru* and *Piper nigrum*. FT-IR spectroscopy, FT-Raman spectroscopy, photoluminescence spectroscopy and UV–Vis absorption spectroscopy are used to characterize the extracted dyes. The dyes are further adopted for Gaussian 09 analysis. The dyes are employed as photosensitizer for titanium dioxide photo-anode based DSSC. The photovoltaic performance of the DSSCs are evaluated under simulated solar light intensity of 100 mW/cm. The solar to electrical energy conversion efficiency of cubebin and betalain pigments and their combination based solar cells are estimated as 0.39 and 0.38%, respectively, which could be attributed to the absorption of natural photosenstizers in wider range of solar spectrum.

Keyword: Dye-sensitized solar cell, Betalain, Cubecin, Photovoltaic performance, Ocimum tenuiflorum, Piper nigrum

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Preparation And Characterization Of Zno Nanopowders By Precipitation Method Using Aqueous Extract From Natural Leaves And Flowers

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Abstract

ZnO nanoparticles have been synthesized by Co-precipitation method from Zinc nitrate using Ethanolic leaf extracts of *Bauhinia variegata*and*Nyctanthes arbor-tristis*which acts as a capping agent. The capping agent acts as a solvent and roles as stabilizer for the synthesis of nano particle. The powder was characterized by X- ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDAX), Photoluminescence Spectroscopy (PL), Fourier Transform Infrared Spectroscopy (FTIR) and UV-Visible (UV-Vis) Spectroscopy. XRD patterns showed that ZnO nanoparticles have Flake-shaped cell structure. SEM pictures reveal the morphology and particle size of prepared ZnO nanoparticles. The compositional analysis of EDAX confirms that prepared ZnO samples are around the nominal composition due to the presence of ZnO. The UV-vis absorption spectrum shows an absorption band at 283 nm due to ZnO nanoparticles which lie much below the bandgap wavelength of 375 nm indicates the monodispersed nature of the nanoparticle distribution. The photoluminescence spectrum exhibits emission peak at 510 nmwhich shows a stronger and green broader visible emission band attributed to the presence of singly ionized oxygen vacancies. FTIR spectrum of the prepared ZnO sample confirms the presence of functional groups and the stretching vibrations of the ZnO nanoparticles. The synthesis method has potential for application in manufacturing units due to ease processing and more economical reagents.

Keyword: Zincnitrate, NaOH, *Bauhinia variegata*and*Nyctanthes arbor-tristis*, ethanol, zinc oxide

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MS69 ISBN NO:9-789388-413282

Effect of surfactant aided barium hydroxide nanoparticles by chemical co-precipitation method

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Abstract

In recent researches, the semiconducting materials have created a great impact due to their physical and chemical properties depending upon their shape and size and also their applications in various fields. Here, the fine powder of surfactant (SDS) aided Barium hydroxide nanoparticles were prepared by chemical co-precipitation method using Barium nitrate, Sodium DeodecylSulphate (SDS) as surfactant, sodium hydroxide pellets and deionised water (solvent). The crystallite size of surfactant aided Barium hydroxide nanoparticles are analyzed using X-Ray Diffraction (XRD) spectrum. The functional groups are identifiedin Fourier Transform Infrared Spectroscopy (FTIR). The surface morphology of the surfactant aided Barium hydroxide nanoparticles is found from scanning electron microscopy (SEM). The optical properties are determined by using UV-visible spectroscopy. Surfactant aidedBarium hydroxide nanoparticlesare extensively used in refining oils and sugar.

Keyword: Barium hydroxide , SDS(Sodium dodecyl sulphate), XRD, FTIR, SEM, UV

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Synthesis and Characterization of Eu:$CaTio_3$ NanoPowder Using Sol-gel Method

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Abstract

The objective is to prepare perovskite type Eu:$CaTio_3$ nanopowder using Sol-gel method. The nanopowder was obtained by low temperature calcinations. The sample was characterized by various advanced techniques. The structural analysis of nanopowder was studied using X-ray diffraction (XRD), while optical absorbance behavior was studied using UV–vis spectrophotometer (UV-Vis),while the composition was studied using Energy dispersive electron spectroscopy (EDS), and the surface morphology was studied using Scanning electron microscopy (SEM). This method is novel, convenient, easy, simple, low cost and effective in comparison to the known methods of the synthesis of nanopowder.

Keyword: Eu:$CaTio_3$, nanopowder, Sol-gel method

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Exploring the structure and Charge density studies of Organic Superconducting Tetrathiafulvalene (TTF) and 7,7,8,8-Tetracyanoquinodimethane (TCNQ) molecule : A DFT and AIM analysis

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Abstract

The bond topological and electrostatic properties of the energetic TTF and TCNQ molecule were carefully evaluated by *ab initio* (HF) and density functional theory (B3LYP) calculations. The optimized (HF/6-311G** and B3LYP/6-311G**) geometric parameters are in excellent agreement with the similar type experimental data. For both levels of calculation, the C–S and C≡N bonds have low charge accumulation at the bond critical point, which indicates that the charges of the bonds are highly depleted compared with all other bonds in the molecule. The bond topological analysis based on the AIM theory shows the difference of charge distribution in all bonds. The molecular conductive properties are solely related to the ESP of the entire system as expected to a little ESP across the system compared with electrode as it has large ESP. For, a good conducting molecule the ESP's are expected to see little along the molecule. The ionization potential gives the very good information of conductivity. These observations give an insight on this kind of super conducting material, which are useful to design navel electronic devices.

Keyword: TTF, TCNQ, *ab initio* (HF) and Density functional theory, AIM

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Thermo chemical, Charge density and Energetic properties of high energetic TNP derivatives via DFT and AIM analysis

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Abstract

Thermo chemical and charge density features, such as atomic charges, bond critical points, and electrostatic potential and explosive properties of TNP [1] derivatives described and compared with reported molecules. The bond topological and explosive properties of the highly energetic tri and tetranitrohexahydro pyrimidine derivatives were carefully evaluated by HF and density functional theory (B3LYP) calculations using Bader's AIM analysis [2]. In this derivatives, the ring adopts a chair conformation, in which the C(1)–N(1)–C(2)–C(3) and C(4)–N(2)–C(1)–H(1) bonds are twisted to an angle -49.2 and 60.7°, confirms, both bonds are gauche oriented. Interestingly, the electron density studies, predicts the C–NO_2 bonds have a low charge accumulation at the bond critical point, which indicates that the charges of the bonds are highly depleted compared with all other bonds in the molecule. The charge accumulation in Car–Nar and N=O bonds is found to be high compared with the NO_2 group attached to C–N bonds; their corresponding high negative $\nabla^2\rho_{bcp}(r)$ confirms its high solidarity. Furthermore, the thermo chemical and sensitivity calculation based on imbalance parameters predicts that the nitro groups attached to C–N and N–N bonds are more sensitive than the other bonds in the molecule and it confirms the NO_2 group attached to C–N and N–N bonds are very weak bonds in the molecule [4]. These bonds may rupture first and initiate the detonation process when the material is exposed to external stimuli. Importantly, the present study also confirms the fair relation between the charge depletion and the bond sensitivity of the molecule.

Keyword: TNP, Density functional theory, AIM, ESP

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Quantum chemical and charge density studies on Gold substituted 8a,9,10,10a-tetrahydro-2,6-Bis-(2-phenylethynyl) anthracene based Nano-molecular Wire

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Abstract

The bond topological and electrostatic properties of the energetic TTF and TCNQ molecule were carefully evaluated by *ab initio* (HF) and density functional theory (B3LYP) calculations. The optimized (HF/6-311G** and B3LYP/6-311G**) geometric parameters are in excellent agreement with the similar type experimental data. For both levels of calculation, the C–S and C≡N bonds have low charge accumulation at the bond critical point, which indicates that the charges of the bonds are highly depleted compared with all other bonds in the molecule. The bond topological analysis based on the AIM theory shows the difference of charge distribution in all bonds. The molecular conductive properties are solely related to the ESP of the entire system as expected to a little ESP across the system compared with electrode as it has large ESP. For, a good conducting molecule the ESP's are expected to see little along the molecule. The ionization potential gives the very good information of conductivity. These observations give an insight on this kind of super conducting material, which are useful to design navel electronic devices.

Keyword: DFT, Electronic structure, Molecular orbital analysis, DOS, DFT, ESP

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Synthesis and Characterization of ZnO Nanoparticles by Precipitation method

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Abstract

ZnO nanoparticles are also known as multi functional nanomaterials are largely synthesized due to its unique physical and chemical properties. In this protocol, Zno nanoparticles are synthesized by the method of precipitation. Since, ZnO nanoparticles have large band gap energy, it is used in semiconductor fabrication. The synthesized samples are characterized using SEM, FTIR, XRD and UV visible spectroscopy studies. The presence of ZnO nanoparticles were confirmed by the FTIR. SEM images show that the surface morphology of Zno nanoparticles are spherical with agglomeration in shape. The crystalline size was analyzed by X-ray diffraction pattern with average size of 22.14 nm and 25.82 nm. The UV analysis shows the calculated band gap energy of Zno nanoparticles are 2.93eV and 4.53 eV.

Keyword: FTIR, SEM, UV, XRD, precipitation method, ZnO Nanoparticles

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TiO_2 photocatalysis: Design and applications

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Abstract

TiO_2 photocatalysis is widely used in a variety of applications and products in the environmental and energy fields, including self-cleaning surfaces, air and water purification systems, sterilization, hydrogen evolution, and photo electrochemical conversion. The development of new materials, however, is strongly required to provide enhanced performances with respect to the photocatalytic properties and to find new uses for TiO_2 photocatalysis. In this review, recent developments in the area of TiO_2 photocatalysis research, in terms of new materials from a structural design perspective, have been summarized. The dimensionality associated with the structure of a TiO_2 material can affect its properties and functions, including its photocatalytic performance, and also more specifically its surface area, adsorption, reflectance, adhesion, and carrier transportation properties. We provide a brief introduction to the current situation in TiO_2 photocatalysis, and describe structurally controlled TiO_2 photocatalysts which can be classified into zero-, one-, two-, and three-dimensional structures. Furthermore, novel applications of TiO_2 surfaces for the fabrication of wettability patterns and for printing are discussed.

Keyword: TiO_2, photocatalysis, adsorption, reflectance, adhesion, carrier transportation

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Preparation of Mo-Cu doped photocatalysts,their photocatalytic and antimicrobial properties

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Abstract

Mo-doped and pure TiO_2 nanoparticles were synthesized using a simple sol-gel method. The prepared catalyst was characterized by XRD, UV-Vis.DRS, TEM, XPS, etc. The effect of metal contents on the photocatalytic activity was investigated. The photocatalytic activity of the doped catalysts was ascertained by the photo-oxidation of acid Rhodamine-B in aqueous solution illuminated with low-pressure mercury lamp (~254 nm). The antimicrobial properties of the modified TiO_2 samples were evaluated with *E. coli* ,Bacillus subtillis and Pseudomonas aeruginosa. It was found that Mo-Cu doped TiO_2 showed better antimicrobial activity in low concentrations. It was found that the modified catalyst showed better photocatalytic degradation than pure TiO_2 in visible light.

Keyword: Photocatalysis, Photo-oxidation, Antimicrobial properties, Rhodamine-B

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The Anodization of Aluminium Metal matrix for Corrosion Protection: An Overview

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Abstract

Aluminium metal matrix composites are gaining widespread attention for over last two decades in various applications such as automobile, aerospace, agriculture farm machinery and many other industrial applications due to its essential properties such as high strength to density ratio, low coefficient of thermal expansion, stiffness, low density and good wear resistance compared to any other metal.Metal matrix composites plays an important role as the binding the reinforcement phases in place and deforming to distribute the stresses among the constituent reinforcement materials under an applied force. The reinforcement of the metal matrix composite improves the stiffness, specific strength, wear, creep and fatigue properties compared to the conventional engineering materials. The reinforcement particles produced more porous structure of the anodized layer for MMC. The aim involved in designing metal matrix composite materials is to combine the desirable attributes of metals.The excellent mechanical properties of these materials and relatively low production cost make them a very attractive candidate for a variety of applications both from scientific and technological viewpoints. The present study deals with the addition of reinforcements such as graphite, fly ash, silicon carbide, red mud, organic material etc. to the Aluminium matrix in various proportions. Each reinforced material has an individual property which when added improves the properties of the base alloy.A comprehensive knowledge of the properties is provided in order to have an overall study of the composites and the best results can be employed for the further development of the Aluminium reinforced composite. The investigation shows that the Aluminium metal matrix composites can be replaced with other conventional metals for better performance and longer life. Hence this review is focused on the aluminium metal matrix composite for corrosion protection in the recent years.

Keyword: Anodization, corrosion protection, Metal-matrix composites, Reinforcement

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Synthesis and Characterisation of Pure Zinc Oxide Nano Particles and Nickel doped Zinc Oxide Nano Particles

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Abstract

In this paper, Zinc oxide nanoparticles are synthesized by simple wet chemical precipitation method. Zinc nitrate and sodium hydroxide are used as the starting materials. Zinc oxide nanoparticles are formed at a very low temperature of the order of 80°C. Nickel doped zinc oxide nanoparticles are synthesized in two steps. In first step precipitate is obtained by reduction of mixture of zinc nitrate, ferric nitrate and starch by Sodium hydroxide solution while in second step the given precipitate is thermally decomposed at high temperature of the order of 400°C. The crystalline of the synthesized nanoparticles is then confirmed by X Ray diffraction Spectroscopy (XRD). The elemental composition of the Powder is detected by Energy Dispersive X-ray spectroscopy (EDAX). The morphology of the Powder is investigated by Scanning Electron Microscopy (SEM). The functional groups present in the nanoparticles where observed by Fourier Transform Infrared spectroscopy (FTIR). The band gap energy was calculated by using Ultraviolet studies (UV).Zinc oxide is a unique material with direct band gap and because of its exceptional optical and electrical properties it has been extensively used in many technological applications such as thin film transistors, gas sensor, biomedical and piezoelectric applications. The magnetic nature present in Nickel doped zinc oxide nanoparticles were mainly used for spintronic applications.

Keyword: Zinc oxide, XRD, EDAX, SEM, FTIR, UV

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Unusual Rheological behavior of Silica-Ionic liquid Nanocomposites as a function of Temperature

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Abstract

Silica-ionic liquid nanocomposite (SINC) has been prepared by dispersing different amounts of silica nanoparticles in Emim TFSI ionic liquid. Dynamic rheological studies on the SINC samples as a function of temperature and concentration (0.5 -5wt %) of silica nanoparticles have been carried out at different temperatures and the elastic modulus of the samples is found to increase upon increasing the temperature. SINC samples with lower concentrations of silica nanoparticles (< 3 wt %) exhibit a weak gel behavior whereas samples with higher concentrations (> 3 wt %) exhibit a strong gel behavior. This transformation is attributed to the formation of more fractal colloidal networks upon increasing the concentration. SINC samples with lower concentrations of silica nanoparticles (< 3 wt %) transform from a weak gel behavior to strong gel behavior upon increasing the temperature. For, samples with higher concentrations of silica nanoparticles (> 3 wt %), gel strength is increased upon increasing the temperature. This behavior of these samples is attributed to the formation more cross-links in fractal colloidal networks upon increasing the temperature.

Keyword: Silica-ionic liquid nanocomposite, Dynamic rheological studies, fractal colloidal networks

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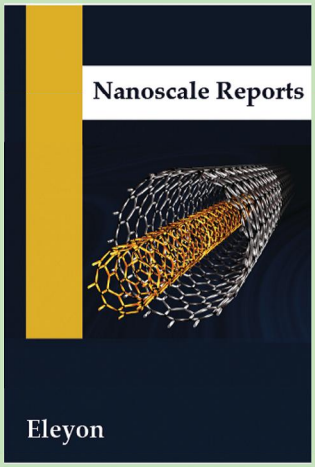

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