

National Conference on Advances in Material Science Research (NCAMSR - 23)

19th & 20th October 2023

Conference Proceedings

**Convener
Dr. S. Uvarajan**

**Organized by
Department of Physics
Thiruvalluvar University,
Vellore**

Sponsored By



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THIRUVALLUVAR UNIVERSITY

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Serkkadu, Vellore - 632 115, Tamil Nadu, India.



MESSAGE

It is a great pleasure and honour for me to invite all the great scientists, academicians, young researchers, delegates and students to the National Conference on Advances in Material Science Research (NCAMSR-23) on 19th and 20th October 2023, organized by the Department of Physics, Thiruvalluvar University, Vellore.

I strongly believe that research, innovation, and collaboration are key to success in a sustainable world. At Thiruvalluvar University, we are dynamically engaged in creating a research environment to promote novel research with a strong application focus in multidisciplinary areas. We are organizing conferences to provide an essential perspective and expertise in continuously emerging trends & practices of arts and science. In the modern era, the evolution of green materials and applications is vital to tackle the environmental problems due to globalization and population. I strongly believe that the NCAMSR-23 will offer an excellent opportunity for the delegates to identify the problems and give an insight into the hot research areas and cutting-edge technologies in materials science.

I appreciate efforts undertaken by the Department of Physics for its commitment and vision towards research. I hope that the conference enriches all with many modern ideas and innovative thoughts that will be fruitful for the researchers in their future endeavours.

I congratulate the team and wish you all the success.

Prof. Dr. T.ARUMUGAM

Vice-Chancellor

Thiruvalluvar University



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MESSAGE

Warm and Happy greetings to all. I am immensely happy that the Department of Physics is organizing two days National Conference on Advances in Material Science Research (NCAMSR-23) on 19th and 20th October 2023.

The theme of National Conference on "Advances in Material Science Research" is very appropriate and I hope that this conference will provide a common platform for the academicians, researchers and industrialists to share their knowledge and experience about recent advancements in the various fields of science and technology.

I appreciate the active interest and participation shown by the faculty members of the Department of Physics in organizing National Level conferences, webinars, and maintaining the research ambience in the Department.

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

Prof. Dr. R.VIJAYARAGAVAN

Registrar i/c.

Thiruvalluvar University



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MESSAGE

It gives me immense pleasure and pride to be a part of the National Conference on Advances in Material Science Research (NCAMSR-23) on 19th and 20th October 2023 organized by the Department of Physics, Thiruvalluvar University.

The motto of the Conference is to bring together experts from academic institutions, industries and researchers for sharing knowledge, expertise and experience in the advances in material science trends. I appreciate the efforts undertaken by the Department of Physics faculty team in organizing the National Conference to create a platform for experts to share and learn.

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

Prof. Dr.M.Chandran

Controller of Examinations (FAC)

Thiruvalluvar University



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MESSAGE

I am extremely happy to know that the Department of Physics, Thiruvalluvar University is organizing a two-days National Conference on Advances in Material Science Research (NCAMSR-23) on 19th and 20th October 2023.

I believe that the conference will provide a useful forum to the participants to share their expertise for extending collaboration in their fields but will also be professionally beneficial to them. It will also help to familiarize the participants on the advanced research happening around the globe.

I wish the organizers a grand success in their endeavour.

Prof. Dr. C. Dhandapani

Dean i/c – College Development Council

Thiruvalluvar University



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Serkkadu, Vellore - 632 115, Tamil Nadu, India.



MESSAGE

It gives me immense pleasure to invite all of you for this magnificent Tamilnadu state Council for Science and Technology Sponsored Two day National level Conference on Advances in Material Science Research (NCAMSR)-23.

It is very delightful to note that this Conference will create a good platform to thrash out the research opportunity in Material Sciences. We have five reputed faculties from reputed institutes will deliver the best outcomes of the theme. I am very much confident that this Conference will bestow Knowledge in relation to Material Sciences which consists of multiple research disciplines, including Nano Materials, Thin films, Ferroelectric materials, Semiconductors, Energy materials etc.

I take this opportunity to wish the paper and poster presenters from various colleges and universities for their successful participation.

I immensely feel happy to thank our Honourable Vice-chancellor and Registrar (i/c) of our Thiruvalluvar University for their support in the conduct of the Two day National level Conference on Advances in Material Science Research (NCAMSR)-23. Also, I thank the faculty members and students for their support to make this Conference a great success.

Dr. S.Uvarajan

Convener (NCAMSR)-23

Head (i/c), Department of Physics

Thiruvalluvar University

Invited Talks

1. Prof. Ranjini Bandyopadhyay

Professor Soft Condensed Matter,
Raman Research Institute,
CV Raman Avenue SadashivaNagar,
Bangalore-560080, India.

2. Prof. A. Sundaresan

Professor & Chair Chemistry and Physics of Materials,
Unit Jawaharlal Nehru Centre for Advanced Scientific Research,
Jakkur, Bengaluru,
Karnataka 560064, India.

3. Prof. K. T. Ramakrishna

Reddy Professor,
Department of Physics,
SVU College of Sciences,
Sri Venkateswara University,
Tirupati, Andhra Pradesh - 517502, India.

4. Prof. N. Arunai Nambi Raj

Professor & Dean School of Advanced Sciences,
Vellore Institute of Technology,
Vellore-632 014, Tamil Nadu, India.

5. Prof. V. Subramanian

Professor & Head Microwave Laboratory,
Department of Physics IIT Madras,
Chennai-600036,
Tamil Nadu, India

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Invited Talks

Invited Talk 1

What are soft materials and why do they flow and deform simultaneously

Prof. Ranjini Bandyopadhyay

Professor,

Soft Condensed Matter,

Raman Research Institute,

CV Raman Avenue Sadashiva Nagar,

Bangalore-560080, India.

This talk introduces concepts connected to the rheology of soft materials. Soft materials such as pastes, gels and foams are ubiquitous and are constituted by macromolecules that interact weakly. As a result, these materials can deform even under thermal stresses and show large responses to even very weak forcing. Rheology refers to the study of the flow and deformation of matter. In this talk, I shall discuss the flow and deformation of familiar soft materials such as silly putty, aqueous foams and suspensions of cornflour upon the application of large shear stresses. I shall demonstrate the intriguing nonlinear flow properties of clay suspensions and granular media under externally imposed forces by discussing some recent experiments performed in our laboratory at the Raman Research Institute.

Invited Talk 2

Superconductivity: A Journey through the Quantum Wonderland

A. Sundaresan

School of Advanced Materials, Chemistry and Physics of Materials Unit,
Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur P.O.,
Bangalore 560064, India.

Superconductivity, a mesmerizing phenomenon in condensed matter physics, has captivated scientists and engineers for over a century. This abstract introduces an enlightening overview talk that explores the intriguing world of superconductivity from its inception to its profound implications. Beginning with a historical perspective, we unravel the milestones in the discovery of superconductivity, from its initial observation in 1911 to the latest breakthroughs in high-temperature superconductors. We delve into the fundamental principles, unveiling the quantum mechanical mechanisms behind this phenomenon, including Cooper pairing and the energy gap. The practical applications of superconductivity are equally astonishing. We navigate its transformative impact on diverse fields, from medical diagnostics with high-field MRI machines to the quest for sustainable energy through superconducting power transmission lines. Moreover, we examine the burgeoning role of superconductors in emerging quantum technologies, promising novel computing and communication paradigms.

Invited Talk 3

Development of $\text{Cu}_2\text{ZnSnS}_4$ Monograin Solar Cells

P. Padma Priyanka¹, P. Babu¹, M. Gapanovich² and *K. T. Ramakrishna Reddy¹

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Currently, there has been much interest on the development of new absorber materials made of earth abundant and non-toxic elements for the development of environmentally safe photovoltaic cells. $\text{Cu}_2\text{ZnSnS}_4$ (CZTS) is one such material that possesses suitable physical characteristics for solar cell development. Flexible and transparent photovoltaic cells are more attracting for a variety of applications, particularly for building integration. Further, monograin cells are more economic and simpler to make than the conventional crystalline cells. The preparation of transparent and flexible CZTS monograin solar cell and its performance is presented. CZTS monograin powder is prepared using the constituent binary compounds in molten CsI as flux material in an evacuated quartz ampoule. The synthesized monograin powders were subjected to chemical treatment using NH_4OH and HCl . The as-grown powders showed Cu_xS and SnO_2 phases in addition to CZTS phase while the chemically treated samples indicated only CZTS phase without any impurity phases. CZTS-based monograin photovoltaic cells were developed using chemical bath deposited CdS as buffer layer on CZTS grains in semi-transparent epoxy film. DC sputtered Al-doped ZnO was coated as the window layer. Finally, indium and silver pastes were used as the contacts to the junction. The initial results on Ag/CZTS/CdS/AZO/In cells showed quantum efficiency of $< 60\%$ and a conversion efficiency of 2.8 %.

Invited Talk 4

Biomaterials in the crossroads of cancer and bone health

N. Arunai Nambi Raj

Dean, School of Advanced Sciences, Vellore Institute of Technology, Vellore-632014,
Tamil Nadu, India

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At the nexus of science, engineering, and medicine, biomaterials are a fascinating and varied area. The main goal of biomaterials is to create materials that can easily integrate with the human body while bridging the gap between artificial materials and live tissues.

Biomaterials for bone regeneration are an essential part of contemporary medicine, providing patients with novel treatments for illnesses resulting in bone abnormalities, injuries, or degeneration. These substances are intended to promote and hasten the body's normal healing processes by creating the right conditions for the growth of new bones.

In cancer research and therapy, biomaterials are used in an array of ways. They allow for precise medication delivery to malignancies, minimising adverse effects and enhancing therapeutic effectiveness. Nanoparticles, which are frequently made of biocompatible materials, precisely target cancer cells. While diagnostic biomaterials and imaging agents improve early cancer diagnosis, biomaterial scaffolds help in cancer biology research and therapy trials. They support innovative therapies including immunomodulation, photodynamic therapy, nano-magnetic hyperthermia, and gene therapy. The treatment and research of cancer are being advanced by this multifaceted discipline.

The advancement and invention of biomaterials has significantly improved patient outcomes, raised quality of life, and increased the potential of contemporary medicine. To meet the ever-evolving difficulties in healthcare, researchers keep pushing the limits of biomaterial science by investigating novel materials and production methods. As science and technology evolve, biomaterials will definitely stay at the cutting edge of medical imaginative thinking, presenting promise for novel remedies that address some of humanity's most laborious ailments.

Invited Talk 5

Magnetoelectric composites and their applications

V. Subramanian

Microwave Laboratory, Department of Physics,
Indian Institute of Technology Madras,
Chennai – 600036

Magnetoelectric composites are a class of devices that operate on the basis of strain transfer between magnetostrictive and electrostrictive materials. The control of magnetostriction, through an external electric field, and control of piezovoltage, through an external magnetic field, can be used to design tunable components, sensors, and energy harvesting applications. The efficiency of these devices depends on the coupling between the magnetostriction and piezoelectricity. In this talk, the basics of magnetoelectric composites will be presented along with some useful applications in the microwave frequency region, magnetic sensing, and energy harvesting.

Oral/Poster Presentation

Abstracts

**Synthesis and Formulation of Nickel Particle Ink for the Fabrication of
Resistance Temperature Detectors (RTDs)**

Arya Narayanan¹, Sumith S², Dr. K. P. Surendran³

¹ M.Sc. Student, Department of Physics, University of Kerala, Thiruvananthapuram.

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ABSTRACT

The flexible resistance temperature detector (RTD) can be considered a powerful device that can be used in various applications, including health monitoring, smart packing, and industrial automation. A flexible, cost-effective, reliable RTD can be fabricated using printed electronics techniques. For the fabrication of RTDs, the nickel particles were synthesized by chemical reduction process. The crystallographic analysis was done by XRD and confirmed the formation of phase pure nickel particles. The morphological analysis was studied using SEM and TEM. A stable screen printable ink was formulated using the synthesized nickel particles in an ethanol-ethylene glycol solvent system. RTD was fabricated by printing formulated nickel particle ink on a flexible Kapton (PI) substrate.

The capability of the printed RTD was demonstrated by measuring its resistive response toward temperature varying from 30° to 120°, and its sensing characteristics, such as linearity, sensitivity, and repeatability were analyzed. It was found that the fabricated Ni RTD shows a linear temperature response with a TCR 0.3% value, which is in good agreement with the already reported Ni RTD values. The flexibility of the printed RTD was verified by studies where we found a negligible change in resistance even after 500 bending cycles. The fabricated wearable sensors have potential application prospects in temperature monitoring.

**Non-Enzymatic Electrochemical Detection Of Fenitrothion Using Graphene
Oxide- Iron Oxide Nanocomposite Modified Gce**

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ABSTRACT

A simple, inexpensive, and effective electrochemical sensor for the detection of fenitrothion (FNT) was fabricated using graphene oxide (GO)/ iron oxide (Fe₃O₄) nanocomposite-modified glassy carbon electrode (GCE). Fenitrothion is an organophosphate insecticide that has been used to control a variety of pests and insects. The morphology of GO sheets synthesized via modified Hummer's method was investigated using SEM and FTIR, whereas that of the Fe₃O₄ nanoparticles synthesized via the co-precipitation method was characterized using XRD, FTIR, and SEM analysis. The formulation of iron oxide and GO nanocomposite was confirmed using EDX, FTIR, and SEM. The preliminary analysis of the GO/Fe₃O₄ modified GCE was done by cyclic voltammetry (CV) and showed an enhanced current response along with a lower reduction potential than the untreated one. This confirms the synergetic effect of GO and Fe₃O₄ nanoparticles in increasing the electrocatalytic properties of the nanocomposite. Further, the analytical study of modified GCE has proceeded using differential pulse voltammetry (DPV). The fabricated sensor exhibits enhanced electrochemical active surface area. A linear correlation between the peak current and FNT concentration is seen in the 6 -70 μM range with a low detection limit of 0.319 μM. Moreover, the sensor offers high selectivity, stability, repeatability, and reproducibility.

**Crystal growth, physico – chemical and quantum chemical investigations on
DAST crystal for optical applications**

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ABSTRACT

The organic molecule of 4-dimethylamino-N-methyl-4-stilbazolium tosylate (DAST) single crystal has been grown by the slow evaporation solution growth technique. We report in this article the synthesis, experimental as well as theoretical investigations of pristine DAST crystal. Powder crystal X-ray diffraction (PXRD) study shows that the grown crystal belongs to a monoclinic crystal system with non-centrosymmetric space group Cc. The Rietveld refinement has been done and compared with the experimental. The spectral analysis of DAST calculations was performed with the help of DFT at the B3LYP/6-311 + G(d,p) basis set level of theory. The experimental results of FTIR and FT-Raman were compared with the computational results. Detailed interpretations of the vibrational spectra were carried out with the aid of vibrational energy distribution analysis using potential energy distribution analysis and vibrational wavenumber scaled by the WLS method. The NBO analysis clearly elucidates the formation of intramolecular H - bonded interaction between π (C₄ - C₅) - π^* (C₆ - C₇) and π (C₆-C₇) \rightarrow π^* (C₈-C₉) and

their energy values are 283.09 and 153.12 (KJmol⁻¹) respectively. The optical properties of the grown crystal were analyzed by UV–Visible studies and compared with theoretical absorption spectral analysis. The second harmonic generation activity of the grown crystal has been tested using an Nd: YAG laser operating wavelength at 1064 nm. Hirshfeld Surface analysis and fingerprint plots was used to determine the intermolecular interactions. Frontier orbital examination revealed the distribution of HOMO and LUMO, while an inverse relationship between first hyperpolarizability and HOMO-LUMO gap suggests efficient molecular orbital overlap, showcasing DAST's potential as an electro-optic material. The first order hyperpolarizability β_0 is a prerequisite to behave as a good NLO material, and the important parameters influencing β generally are donor–acceptor system, nature of substituents, conjugated π system and the influence of planarity. The results also show that the titled compounds studied in our research are good NLO and potential electro-optic materials.

Keywords: Crystal growth; vibrational analysis; DFT study; NBO; Hirshfeld Surface; Linear and non-linear optical property;

Structural and optical properties of Zn doped Cobalt ferrite nanoparticles

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ABSTRACT

The hydrothermal approach was used to create the nanostructured zinc-doped cobalt ferrites. XRD, FTIR, UV-Vis, and FESEM, the produced nanoparticles were further characterized. Spinel ferrite's composition and structure were validated by XRD analysis. The nanoparticles' aggregated and spherical structure is verified by FE-SEM. FTIR was used to confirm the vibrational stretching modes of the tetrahedral (536 cm^{-1}) and octahedral (461 cm^{-1}) sites. The optical energy band gap proves that each sample contained visible active components.

Key words: XRD, FTIR, UV-Vis, FE-SEM, and Hydrothermal

**Sunlight Assisted Photodegradation of methylene blue Using Green Synthesized
ZnO Nanoparticles**

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ABSTRACT

Zinc oxide nanoparticles (ZnO NPs) have been successfully produced through an eco-friendly method using the aqueous extract of *PileaMicrophylla* leaves. This green approach harnesses the natural phytochemicals present in *Raphanussativus* (radish) leaves extract, serving as both reducing and stabilizing agents. This innovation eliminates the need for expensive solvents and hazardous chemical agents, promoting a safer and more sustainable synthesis process. The green synthesized ZnO nanoparticles were characterized by UV-Visible spectroscopy (UV-Vis), Fourier transforms infrared spectroscopy (FT-IR), and X-Ray diffraction (XRD) analysis. From the UV-Vis analysis. The FT-IR spectroscopy confirms the phytochemicals in *PileaMicrophylla* involved in nanoparticle synthesis and stabilizing agents. The XRD analysis shows that ZnO nanoparticles were present in the synthesized nanoparticles, which was confirmed by JCPDS card No. 89-1397. The photocatalytic efficiency of synthesized ZnO NPs was confirmed by photocatalytic degradation of organic pollutant dye under sunlight in the absence of hydrogen peroxide (H₂O₂). The photocatalytic degradation of MB dye was monitored by UV-Vis spectroscopy with different time intervals.

**Ecological risk evaluation and heavy metal contamination in sediments on the
Tamilnadu South East Coast, India with a statistical method**

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ABSTRACT

The purpose of the study is to determine the concentrations of heavy metals and ecological risk in the sediment samples collected from Poombuhar to Karaikal along the Tamilnadu South East Coast using the ICP-MS technique. The sample is total digestion using Nitric / Hydrochloric acid mixture (Aqua Regia) in microwave digester unit according to EPA Method 200.2 and Method 3050. The sample was digested with a ramp time of ten min, using 1600 w power. All digests were filtered through 0.45 μm PTFE filter and with ultrapure water after cooling to room temperature, and stored at 4 $^{\circ}\text{C}$ in polyethylene vials until analysis. The samples were investigated using Inductively Coupled Plasma Mass Spectrometry (ICP-MS) (Agilent: 7700x). The Sediment Quality Guidelines (SQGs) are used to assess the eco toxicological value of toxicity from heavy metals. The multivariate statistical analysis is applied to find out the source of origin of metals from anthropogenic input or natural sources. Factor and cluster analysis identified the sources of pollution. The heavy metals Cr, As, Zr&Pb observed high concentration in PKK-3 when compared to other locations, and this can be ascribed as anthropogenic activities. Pollution indices like Enrichment factor (EF), Contamination facto, Geo-accumulation index (I_{geo}) and metal pollution load index (PLI) were computed to measure the level of pollution and contamination status in the study area. The computed EF, I_{geo} , CF and PLI values showed considerable pollution by Pb& Zn in the sediments, and it is due to the industrial activities, and vehicle emissions denoted the most significant sources of the pollution. Further the analysis of SQGs revealed that there no severe pollution of the East Coast of Tamilnadu.

Keywords: Sediment, heavy metal, pollution indices, statistical analysis.

A DFT+U study of barium based double perovskite oxide $\text{Ba}_2\text{TiMoO}_6$

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ABSTRACT

A density functional theory plus Hubbard potential (U) approach is used to study the structural, electronic and magnetic properties of barium based double perovskite oxide ($\text{Ba}_2\text{TiMoO}_6$). In the aspect of stability, formation energy of the compound is calculated and has been found to be thermodynamically stable in ground state. Volume optimization curve showcase the compound is more stable in ferromagnetic phase compared to non-magnetic phase. Band structure and DOS are calculated which reveal the half-metallic ferromagnetism of the double perovskite system exhibiting 100 percent spin polarization at the Fermi level E_F . This result proposes the investigated compound could be used in spintronics applications.

Keywords: DFT+U method; Doubleperovskite; Half-metallic nature; Magnetic moment; spintronics

**Luminescent Properties of CaS AND $\text{Ca}_x\text{Sr}_{1-x}\text{S}:\text{Eu}$ Red Emitting Sulfide
Phosphors**

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ABSTRACT

Europium doped red emitting CaS and $\text{Ca}_{(1-x)}\text{Sr}_x\text{S}$ phosphors were synthesized by solid state reaction in CO reducing atmosphere at 1100°C for 2h. The synthesized phosphor was excited in the visible region and red emission occurred with single broadband. Photoluminescence (PL) emission intensity of CaS:Eu was studied with different monovalent fluxes and by varying Ca/Sr concentrations. PL intensity of the synthesized phosphor was higher with KCl flux. The emission wavelength of the $\text{Ca}_x\text{Sr}_{1-x}\text{S}:\text{Eu}$ phosphor shifted from 647 nm to 623 nm with Ca concentration x from 1 down to 0. Thermoluminescence study reveals that major TL peak on UV irradiation occurred at 90°C with shoulders at 145°C and 310°C and observed major TL glow peak at 98°C on X-ray irradiation. An additional weak TL peak occurred at 156°C and 305°C. CIE indicates that the emission colour of the CaS:Eu²⁺ phosphors were located in the red region hence this phosphor was implanted in blue LED along with YAG:Ce as red phosphor to produce white light. Emission wavelength was varied from 623 nm to 647 nm by adjusting Ca/Sr ratio.

Advancements in Medical Image Processing for Disease Detection and Diagnosis

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ABSTRACT

Medical image processing has witnessed remarkable progress in recent years, offering transformative potential in healthcare. This paper presents an overview of cutting-edge developments in medical image processing, with a primary focus on its application in the detection and diagnosis of diseases. Utilizing advanced techniques like deep learning, computer vision, and image segmentation, this research explores the analysis of various medical images, including X-rays, CT scans, MRI scans, and histopathological slides. One of the central themes of this paper is the emergence of deep neural networks for tasks such as image classification and object detection. These networks have shown exceptional promise in automating the interpretation of medical images, providing accurate and rapid assessments of anomalies. Furthermore, the paper delves into the importance of image segmentation techniques, enabling precise localization and characterization of regions of interest within images. A critical aspect of the discussed advancements is their applicability across diverse medical imaging modalities. Researchers have made significant strides in the fusion of multi-modal images, enhancing diagnostic accuracy by leveraging complementary information from different imaging sources. This synergy has proven particularly valuable in the detection of complex conditions and the tracking of disease progression. Despite the tremendous potential, challenges persist in the field of medical image processing. The paper addresses the need for extensive and meticulously annotated datasets, which are essential for training robust deep learning models. Additionally, ethical considerations regarding patient data privacy and security are paramount, requiring stringent safeguards in image acquisition, storage, and sharing. These concerns are addressed alongside insights into potential solutions. This research paper also emphasizes the growing role of medical image processing in telemedicine. The ability to transmit medical images remotely,

combined with real-time processing, has the potential to revolutionize healthcare delivery. Telemedicine applications enable timely consultations, especially in remote or underserved areas, thus broadening access to expert medical care.

In conclusion, this paper underscores the transformative impact of medical image processing on disease detection and diagnosis. Through the integration of advanced technologies and the collaboration of multidisciplinary teams, medical image processing has become an indispensable tool in modern healthcare. By overcoming challenges, respecting ethical considerations, and embracing telemedicine, we can harness the full potential of these innovations to enhance patient outcomes and advance the practice of medicine.

Keywords: Medical Image Processing, Deep Learning, Computer Vision, Image Segmentation, Disease Detection, Diagnosis, Multi-modal Imaging, Telemedicine, Data Privacy.

Synthesis of Ti DOPED ZnO/SnO₂-Nanocomposite and Their Photocatalytic Properties

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ABSTRACT

A simple chemical precipitation method to synthesize ZnO/SnO₂ nanostructures has been investigated in the presence of Ti as a dopant for highly efficient photocatalyst. The synthesized samples were characterized through X-ray diffraction, UV-Vis Diffuse Reflectance Spectroscopy; Field Emission Scanning Electron Microscopy, Transmission Electron Microscopy. The photocatalytic activity of the samples was tested using the degradation of MB under sun light as model reaction. The structural investigation indicated that the XRD patterns reveal highly crystalline ZnO/SnO₂ nanoparticles. The newly prepared Ti doped ZnO/SnO₂ nanostructures have been evaluated for photodegradation of methylene blue (MB) under visible light. The photodegradation of MB proceeds much more rapidly in the presence of Ti doped ZnO/SnO₂ compared to the undoped ZnO/SnO₂ nanoparticles. These results indicate that Ti doped ZnO/SnO₂ nanostructures are very promising to fabricate highly efficient photocatalysts.

Keywords: nanostructures, photocatalysts, photodegradation, methylene blue

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**Synthesis, Characterisation and Enhanced Photocatalytic Activity of
TiO₂/ZnO Binary Nanocomposites**

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ABSTRACT

Researchers highlight the field of nanosized semiconducting oxide Waste water treatment because of threats to the atmosphere and health of humans. In this work, TiO₂/ZnO nanocomposites were synthesized via the method of simple chemical precipitation. The products were characterized with powder X-ray diffraction (XRD), thermogravimetric and differential thermal analysis (TG-DTA), UV-Vis diffuse reflectance spectroscopy (UV-Vis DRS) and Brunauer-Emmett-Teller measurement of specific surface area, which showed that TiO₂-ZnO nanostructured composites were obtained with zinc oxide. Besides, modification of a commercial sample with zinc oxide led to a slight decrease in the specific surface area, while modification of a synthesized-by-simple chemical precipitation method TiO₂ sample led to an increase. It was found that sorption properties of the obtained nanocomposites and pure TiO₂ are better towards MB dyes. It was established that in terms of photocatalytic activity, TiO₂-ZnO nanocomposites are more promising than solid solutions, and modification of TiO₂ with zinc oxide, in general, leads to improvement of its photocatalytic activity.

Keywords: nanocomposites, photocatalytic, chemical precipitation, semiconducting oxide

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**Construction of BiVO₄/LDH Heterostructure with Enhanced Photocatalytic
Performance Under Visible-light**

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ABSTRACT

A bismuth vanadate (BiVO₄) with a cocatalyst consisting of layered double-hydroxide (LDH) nanoparticles was fabricated by a one-step hydrothermal route, employed for the photocatalytic RhB degradation under visible light exposure. LDH nanoparticles can improve light-absorption capacities and facilitate efficient e⁻-h⁺ transfer to the heterosurface. All the samples were characterized using XRD, SEM, TEM, EDS, UV-DRS, PL, and photoelectrochemical studies. The photocatalytic ability and recyclability of the BiVO₄/LDH photocatalyst demonstrate the composite shows high structural stability. The improved photocatalytic activities were attributed to the high adsorption to RhB, the stability of the heterostructure, and the energy level that facilitates the migration and separation of charge carriers.

Investigation of Photocatalytic Degradation of An Organic Pollutant Methylene Blue Using Ag Doped Zinc Vanadate Nanoparticles Synthesized By Hydrothermal Assistant Co-Precipitate Method

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ABSTRACT

Ag doped zinc vanadate(Ag-Zn₂V₂O₇) nanoparticles were prepared by doping silver at 2, 4 and 6Wt% with the zinc vanadate using hydrothermally assist co-precipitation method. Doping of Ag improves the crystalline nature of zinc vanadate by reducing the crystallite size is confirmed with X-Ray diffraction analysis. Alteration in the microstructure of the zinc vanadate is analysed using the SEM images. EDS spectra confirms the presence of silver in the synthesised nanoparticle. The XPS survey of Ag doped α -ZnV₂O₇ reveals the presence of Zn, V, O, and Ag without any impurities except a small amount of absorbed carbon. The absorption spectrum used to find the bandgap of the synthesised nanoparticles. The light absorption behaviour of the prepared nanoparticles are studied with the help of Uv-Visible spectrum and Photoluminescence analysis. The photodegradation percentage of the methylene blue dye by solar energy raises doping of silver incorporation of silver in the zinc vanadate.

Keyword: Photocatalytic, Methylene blue, PL, Zinc Vanadate.

The effect of Barium doping in SmAlO₃ (Ba= 1%, 3%,5%) on Structural, morphological and Dielectric properties: Ball milling Technique

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ABSTRACT

Perovskite oxides have been attracted by researchers due to their applications in different fields. Accordingly, samarium aluminate (SmAlO₃) and Ba-doped SmAlO₃ ceramics were prepared from a mixture of BaCO₃, Sm₂O₃ and Al₂O₃ powders by the ball milling technique. The structural and morphological properties are measured by various characteristic techniques such as powder X-ray diffraction, Fourier transform infrared spectrophotometer (FTIR), field emission scanning electron microscopy (FE-SEM) and energy-dispersive X-ray spectroscopy (EDS). Changes in structural properties due to Ba²⁺ doping in the Sm³⁺-site are confirmed with Rietveld refinement using GSAS software. The metal oxide vibrational bands were found around 660 cm⁻¹ by the FTIR analysis. The FE-SEM results suggested that the grain size decreased while increasing Ba doped (1%,3%,5%) on samarium aluminate. As obtained from the EDS analysis, it is seen that Sm, Ba, Al and O components are homogeneously distributed throughout the structure, which was also in accordance with EDX. Dielectric constant and loss tangent are measured with various frequency ranges for SmAlO₃ and Ba:SmAlO₃ samples.

Keywords: Ba:SmAlO₃, ball milling technique, Rietveld refinement, EDS analysis

**Transition Metal Dichalcogenide Based Electrochemical Sensor for the Detection
of the Pesticide Carbofuran**

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ABSTRACT

The pesticide carbofuran (CF), also known as 2,3-Dihydro-2,2-dimethyl-7-benzofuranol N-methylcarbamate, is extensively used as a systemic insecticide, nematicide, and acaricide for home, industrial, and agricultural reasons. It is advised in the planting of cotton, sugar cane, bananas, coffee, and other crops. CF and its metabolites, damage food, surface water, and ground water as a result of their widespread use. The acetylcholinesterase activity of CF makes it extremely toxic to fish, animals, birds, and other species. Endocrine disturbance, abnormalities of the reproductive system are all associated with CF in humans. CF is prohibited in Canada and the EU and was classified as a dangerous substance by the US in 2008. However, some developing nations continue to utilize it.

CF environmental purification is of the utmost importance and urgently calls for an appropriate and effective corrective method. Therefore, it is vital to develop an easy, low-cost, speedy, and reliable method for detecting CF in food and environmental samples at low concentrations. CF has been detected utilizing difficult, expensive, and time-consuming processes that frequently require pre-treatment of the samples. On the other hand, electrochemical methods offer high sensitivity, selectivity, and quick detection at a low concentration. As a result, numerous electrochemical sensors have been described with electrodes modified utilizing various materials. A large surface area of nanomaterials enables increased loading capacity and reactant mass transfer, both of which are advantageous for signal amplification.

TMDs, a type of 2D inorganic materials composed of chalcogen elements and transition metals from groups 4 to 7, have been investigated for use in a variety of applications, including optoelectronics, photovoltaics, spintronics, energy storage, and catalysis. However, electrochemical sensing has gotten less attention. Molybdenum disulfide (MoS_2) nanosheets, a type of TMD, have attracted increased attention as a result of their vastly different electrical, physicochemical, biological, and mechanical properties. More adsorption sites are created by the 2D stacked nanosheets of MoS_2 , which further enhances the sensor-defining characteristics. We used a hydrothermal approach to create 2D Molybdenum Disulfide (MoS_2) nanosheets for the current work. CF detection and quantification are made possible by the developed electrochemical sensor that includes MoS_2 modified glassy carbon electrode (MoS_2/GCE) as its working electrode. Through cyclic voltammetry (CV) experiments, the lower limit of detection, sensitivity, selectivity, and practical utility are assessed.

Structural and Optical Properties of Zinc Oxide Nanoparticles

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ABSTRACT

Zinc Oxide Nanoparticles were synthesized by Chemical precipitation method. The synthesized Nanoparticles were calcined at 400 °C to get nano crystalline phase. The synthesized ZnO powders were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Photoluminescence (PL) spectroscopy, Field emission scanning Electron microscopy (FE-SEM), Energy dispersive x-ray analysis (EDX), finally, the current study has clearly demonstrated that the particle size variations and surface area to volume ratios of ZnO NPs are responsible for significant higher antibacterial activities. Further, the present investigation suggests that ZnO NPs has the potential applications for various medical and industrial fields so, that the investigation is so useful and helpful to the scientific communities.

Keywords: ZnO,Structural, Morphology and Photocatalytic activities.

**Bio-Synthesis of Copper Oxide Nanoparticles using *VitexNegundo* leaf Extract
and its Antibacterial Activity**

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ABSTRACT

In this present study, copper oxide nanoparticles was synthesized using an aqueous extract of the *VitexNegundo* leaf as a stabilizing and capping agent, and they were prepared using Bio synthesis method. The synthesized copper oxide nanoparticles were characterized by the following techniques such as TGA, XRD, FT-IR and SEM. According to TGA, the calcination temperature of synthesized copper oxide nanoparticles was found to be 600°C. Based on XRD results, the copper oxide nanoparticles occur in a monoclinic geometry, and the average crystallite size of the copper oxide nanoparticles was found to be 30 nm. The peak at 605, 510 & 486 cm^{-1} is due to the vibration of Cu-O bond from FT-IR analysis. The synthesized copper oxide nanoparticles were subjected to antibacterial activity by agar-well diffusion method.

Keywords: Copper oxide NPs, Leaf extract, Anti-bacterial activity

Photocatalytic Degradation Of Azo Dye By Using MnO₂@ZnO

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ABSTRACT

The photocatalytic degradation of an azo dye Trypan Blue (TB) using MnO₂@ZnO composite catalyst. The MnO₂@ZnO composite catalyst was prepared by the sol-gel process aided by ultrasound method. The photocatalytic activity of MnO₂@ZnO was investigated for the degradation of an azo dye, Trypan Blue (TB) in aqueous solution has been investigated under solar irradiation. The blank experiment for either illuminated Trypan Blue (TB) solution or the suspension containing MnO₂@ZnO and Trypan Blue (TB) in the dark showed that both illumination and the catalyst were necessary for the destruction of Trypan Blue (TB). The photocatalyst of MnO₂@ZnO was characterized by XRD, TEM, FE-SEM, EDX, UV-DRS, and PL spectrum. The effects of operational parameters such as the amount of photocatalyst, dye concentration and initial pH have been examined. The mineralization of Trypan Blue (TB) has been confirmed by COD and hydroxyl radical drastic analysis measurements have been discussed under solar light.

**Green Synthesis of CuO Nanoparticles Using Leaf Extract Its Application For
Photocatalytic Activity**

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ABSTRACT

In this research study, the sustainable and eco- friendly green synthesis report on the use of plant extract alternate to chemicals was discussed. The *Cardiospermumballicacabum* extract was used as a natural reagent to synthesize nanoparticles a brief discussion on the usage of plant extract were also summarized. Copper Oxide nanoparticles (NPs) were successfully prepared using a simple way involving the combination reaction between copper nitrate and leaf extract. The synthesis under leaf extract response played an important role and led to the formation of copper oxide NPs of different size and shapes. The catalyst was characterized by XRD, FTIR, UV–Vis–DRS, PL, SEM with EDX and TEM analysis. The crystalline structure and phase identification was examined using XRD analysis; The results suggested that the nanocatalyst CuO has potential applications as an efficient catalytic material with high efficiency for the photocatalytic degradation of organic pollutants in aqueous solution under UV light irradiation.

Keywords: CuO, *Cardiospermumballicacabum* and Photocatalytic Activity

**Synthesis, Characterization and Efficient Photocatalytic Activity of Hydrothermally
Synthesized CeO₂ Nanoparticles**

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ABSTRACT

The CeO₂ nanoparticles were synthesized by effective hydrothermal method. The CeO₂ nanoparticles have been characterized by X-ray powder diffraction (XRD), High resolution scanning electron microscopy (HRSEM), Energy dispersive X-ray spectroscopy (EDX), transmission electron microscopy (TEM) and Ultraviolet visible spectroscopy. The nanocrystalline size and strain of the CeO₂ nanoparticles have been inspected by Williamson-Hall analysis. The quantum size effect outcomes in spectacular variation in the optical and vibrational appearances of nanostructured materials likened to their bulk counterparts. Functional tests of CeO₂ nanoparticles include photocatalytic effect in the degradation of methylene blue.

Keywords: CeO₂, Structural, Morphology and Photocatalytic activities.

**Photostimulated and Thermostimulated Luminescence Mechanisms in BaFBr:Eu²⁺
X-ray Storage Phosphor**

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ABSTRACT

The synthesis of the technologically important BaFBr:Eu²⁺x-ray storage phosphor using decomposition reaction in air at 400°C followed by sintering in reduced atmosphere at 850°C is reported. Its photoluminescence (PL) emission occurs at 390 nm (λ_{emi}) on excitation at 330 nm (λ_{exi}). On x-irradiation, its photostimulated luminescence (PSL) emission and stimulation occur at 390 nm (λ_{emi}) and 567 nm (λ_{sti}) respectively. It showed the incorporation of Eu²⁺ into the BaFBr lattice. The Eu concentration, molar ratio of the constituents, dose vs PSL response were studied. Fluorine excess non-stoichiometric BaFBr:Eu²⁺ resulted in a higher PSL sensitivity. It is proposed that on x-irradiation, electrons released from interstitial fluorine ions get trapped at bromine ion vacancies and on photo-stimulation, electrons released from F(Br⁻) centres recombine with F₂⁻ molecular ions and decay under Eu²⁺ (390 nm) emission. Correlation studies of PSL and thermoluminescence (TL) revealed that the defects causing the 126°C TL peak and those giving rise to PSL in BaFBr:Eu²⁺ are the same.

Keywords: BaFBr:Eu²⁺, photostimulated luminescence, emission and stimulation spectra, dose response, correlation of PSL with TL.

Facile Green Synthesis of Zinc Oxide Nanoparticles and Its Photocatalytic Activity

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ABSTRACT

In this present study, Zinc oxide nanoparticles was synthesized using an aqueous extract of the *Cardiospermumballicacabum* leaf as a stabilizing and capping agent, and they were prepared using Bio-synthesis method. The synthesized Zinc oxide nanoparticles were characterized by the following techniques such as TGA, XRD, FT-IR and SEM. According to TGA, the calcination temperature of synthesized Zinc oxide nanoparticles was found to be 450°C. Based on XRD results, the Zinc oxide nanoparticles occur in a monoclinic geometry, and the average crystallite size of the Zinc oxide nanoparticles was found to be 35 nm. The synthesized Zinc oxide nanoparticles were subjected to Photocatalytic Activity

Keywords: Copper oxide NPs, Plant extract and Photocatalytic Activity

Investigations on the Effect of Shock Waves on Morphology of Silver Nanofluids

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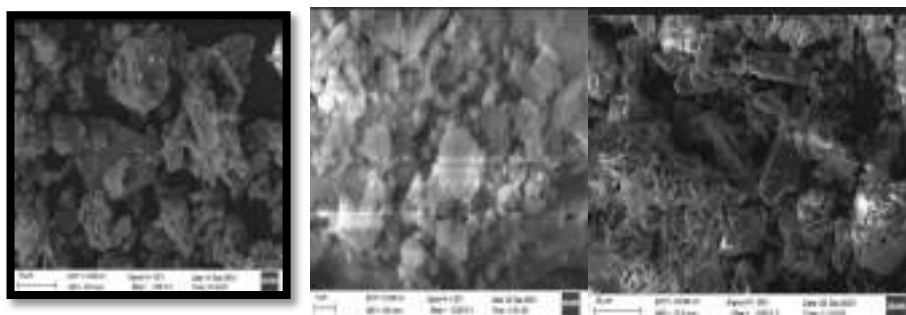
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ABSTRACT

The Present work demonstrates the finding on the effect of shockwave on Silver Nano fluids (AgNfs). Silver Nano fluid was prepared by hydrothermal method using Trisodium citrate as a reducing agent. The test material of AgNfs was loaded with 50 and 100 shock pluses with Mach number 2.2. Control and shock loaded samples were analyzed by SEM (scanning electron microscope), UV-Vis (Ultraviolet visible Spectroscopy), FT-RAMAN (Fourier Transform Raman spectroscopy), Fluorescence, Dynamic Light Scattering (DLS) and KD2 Pro -thermal conductivity measurements. The UV – Visible Spectrum of shock wave loaded AgNfs have absorption Peak at around 420-500 nm. The SEM image shows that the particles were dispersed by increasing number of shockwaves. Dynamic light scattering shows that particle size is around 100 nm. Thermal conductivity increases for shock loaded AgNfs than control. It was analyzed that AgNfs very good florescence properties. The morphology florescence and thermal conductivity are changed for the 100 shocked sample the new florescence peak indicates that the shock loaded AgNfs may have potential application.

Keywords: Hydrothermal, Siver Nitrate, Trisodium citrate, Shock waves.



SEM Images of Control, 50 and 100 shock loaded AgNf

**Green Synthesis of Silver Nanoparticles using Plant Extract Tribulus Terrestris
and their Antibacterial and Antioxidant Activities**

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ABSTRACT

In current years, the sustainable approach of synthesizing silver nanoparticles (AgNPs) has gained much interest among researchers. The flora of the Indian field is rich with a variety of medicinal plants that have the potential to include various sources of effective, cost efficient, non-toxic, environmentally safe reducing and stabilizing compounds that can be utilized in synthesizing in AgNPs. Here, in this study, the author investigates an efficient and sustainable route of AgNP preparation from 1 mM aqueous AgNO₃ using leaf extracts of Tribulusterrestris well enriched for their vast availability and therapeutic property against Urinary Tract Infections (UTIs) samples.

Keywords: Nanoparticle, Antimicrobial Activity, Antioxidant activity, DPPH assay, Plant extract

GSM Based Voting Machine

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ABSTRACT

Elections are the cornerstone of democratic societies, allowing citizens to express their preferences and choose their representatives. However, traditional voting methods have often faced challenges such as inefficiency, inaccessibility, and the potential for fraud. To address these issues, a groundbreaking solution has emerged in the form of the GSM-Based Voting Machine. The Global System for Mobile Communications (GSM) has transformed the way we communicate, and now it is poised to revolutionize the electoral process. This innovative voting system leverages mobile technology to provide a secure, efficient, and accessible platform for citizens to vote. Here, we delve deeper into the features, benefits, and implications of the GSM-based voting machine.

Remote Accessibility: One of the primary advantages of the GSM-based voting machine is its ability to enable remote voting. Traditional voting requires citizens to visit specific polling stations, often resulting in long queues and logistical challenges. With this system, voters can participate in elections from the comfort of their own homes or any location with cellular network coverage. This eliminates the need for physical polling stations and the associated travel inconveniences, making the voting process more convenient and accessible.

Real-time Data Collection: The system's integration with GSM technology allows for real-time data collection. As voters cast their ballots electronically, the results are recorded and transmitted instantaneously. This real-time data collection significantly reduces the time required for tallying and tabulating votes, providing election officials and the public with prompt and accurate results. This enhances the efficiency of the electoral process and helps build trust in the transparency of elections.

Enhanced Security: Security is a paramount concern in any voting system. The GSM-based voting machine addresses this concern through robust security measures. It incorporates secure authentication protocols and encryption to safeguard the integrity and confidentiality of

the voting process. Each vote is encrypted and securely transmitted to a central database, minimizing the risk of tampering or fraudulent activities. This heightened security ensures the legitimacy of the electoral outcomes. Cost and Time Efficiency: Traditional paper-based voting systems involve significant costs related to the printing of ballots, setup of polling stations, and manual counting of votes. The GSM-based voting machine offers a cost-effective alternative by eliminating the need for physical ballots and reducing the operational expenses associated with traditional elections. Moreover, the time required for the election process is substantially reduced, as there is no manual counting involved. This efficiency not only saves resources but also minimizes the potential for errors or delays in delivering election results. The GSM-Based Voting Machine represents a significant step forward in the evolution of electoral systems. Its potential to revolutionize the way elections are conducted cannot be understated. By leveraging GSM technology, this system offers a secure, efficient, and accessible means of casting votes, ultimately strengthening the democratic process. It simplifies the voting experience for citizens, reduces costs, and enhances transparency. While challenges such as digital literacy and network coverage in remote areas need to be considered, the long-term benefits of adopting this technology are substantial.

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**Assessment of Heavy Metal Contamination in Marine Sediments of East Coast of
Tamil Nadu Affected by Different Pollution Sources**

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ABSTRACT

The aim of this study was to determine the concentration of heavy metals in the sediments of Periyakalpet to Parangipettai coast, east coast of Tamil Nadu, by using energy-dispersive X-ray fluorescence (EDXRF) technique. X-ray fluorescence spectroscopy is applied to determine the concentration of essential and toxic heavy metals such as silicon (Si), potassium (K), calcium (Ca), titanium (Ti), iron (Fe), copper (Cu), zinc (Zn), nickel (Ni), and lead (Pb) in the sediments of study area. The average heavy metal concentrations in the sediment samples were found in the order Al > Fe > Ca > Ti > K > Mg > Mn > Ba > V > Cr > Zn > La > Ni > Pb > Co > Cd > Cu. The average heavy metal concentrations were below the world crustal average. The degree of contamination by heavy metals was evaluated using pollution indices. The results of pollution indices revealed that titanium (Ti) and cadmium (Cd) were significantly enriched in sediments. Pearson correlation analysis was performed among heavy metal concentrations to know the existing relationship between them and also the findings indicate that anthropogenic sources such as boating and tourism activities have a probable contribution on the enrichment of K, Ca, Ti, Fe, Cu, and Pb in sediments, necessitating more attention in monitoring of toxic heavy metals (such as Pb) contamination in the coastal environment.

Keywords: Sediments, EDXRF, Heavy metals, Pollution indices, Multivariate statistical method.

**Green Synthesis And Characterization of Copper Nanoparticles by Leaf Extract
of *Pergulariya Tomentosa***

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ABSTRACT

Development of green technology is generating interest of researchers towards ecofriendly and low-cost methods for biosynthesis of nanoparticles (NPs). In this study, copper oxide (CuO) NPs were synthesized using a copper nitrate trihydrate precursor and *pergulariyatomentosaleaves* extract as a reducing and capping agent during the synthesis. In this investigation, *Pergulariatomentosaleaves* were used as a promising source of bioproducts for the reduction of copper sulfate into copper oxide nanoparticles. The prepared nanoparticles were characterized using Fourier-transform infrared spectroscopy (FT-IR), X-Ray Diffraction (XRD), Transmission electron microscopy (TEM).

Effect of Shock Waves on Polycrystalline Sample of L-Methionine Maleate

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ABSTRACT

Analysis of impact of shock wave on Polycrystalline material of L-Methionine maleate was studied. L-Methionine maleate (LMM) powder crystal, has been grown by slow evaporation method from aqueous solution from amino acid family. Few optically clear and well-shaped crystals were obtained in a period of two months. After the shock tube calibration, the synthesized powder crystal was taken in the sample holder and the shock waves with Mach number 2.2 were loaded for shocks 100, 200 and 300 times. From the shock loading experiment it was confirmed that the crystal was stable under shocked conditions. Single crystal X-ray diffraction studies were carried out to confirm the structure with that of existing one and lattice parameters of the grown crystal were determined. FTIR studies confirm the presence of functional groups of L-Methionine Maleate. A DRS study reveals that the grown crystal has 100% of reflectance and transmittance. The details will be presented.

Keywords: L-Methionine Maleate, Shock wave, XRD, FTIR, DRS.

**Design of Biostable Collagen Resistance Against Collagenolytic Degradation by
Clostridium Histolyticum Collagenase**

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ABSTRACT

In this study, we have prepared the biostable collagen scaffold which is crosslinked by dialdehyde chitosan (DAC) with presence of Gallic acid (GA) and characterized its physico-chemical, biostable and biocompatible properties. The dialdehyde groups from DAC crosslinked with collagen functional groups that increase the molecular crosslinking owing to the large number of amino groups in its molecular chain. This scaffold exhibited 87% resistance against collagenolytic degradation by clostridium histolyticum collagenase. The results showed that the improved biostability which prevents the free access of the collagenase to binds with the collagen triple helical chains. This scaffold confirms high biocompatibilities, enhanced cell proliferation and adhesions properties. This result gains new insight into the collagen scaffold to improve the biostability against microbial collagenase. This could be a suitable method to prepare collagenous biomaterials for industrial and biomedical applications.

Keywords: Collagen; Dialdehyde chitosan; Gallic acid; Scaffold; Biostable.

**Green Synthesis of Copper Oxide Nanoparticles from *Wrighitiatinctoria* Leaf
Extract for Reduction of Nitro Compounds**

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ABSTRACT

In this present study we have synthesized copper oxide nanoparticles (CuO NPs) using *Wrighitiatinctoria* leaf extract as reducing stabilizing agents. The prepared nanoparticles were characterized by UV-vis spectroscopy, FT-IR spectroscopy, XRD and zeta potential analysis. The FT-IR results showed the phytoconstituents responsible for the reduction and capping agents for the synthesis of nanoparticles. The average crystallite size was found to be 21.4 nm using Scherrer equation. The stability of the CuO NPs was analyzed by zeta potential and found to be -24.2 mV. The green synthesized CuO NPs were utilized for the reduction of 4-nitrophenol by using sodium borohydride as a reducing agent. The rate of the reaction was calculated to be $1.1 \times 10^{-4} \text{ sec}^{-1}$ and follows pseudo first order kinetics. The formation of 4-aminophenol was confirmed by Ninhydrin test. The results indicated that the green synthesized CuO NPs showed good catalytic activity.

Keywords: Green synthesis; CuO NPs; 4-nitrophenol; 4-aminophenol.

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**Manganese Chloride doped Itaconic acid single crystal: A promising third order
NLO material for photonic applications**

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ABSTRACT

This research work discusses the effect of doping manganese chloride in itaconic acid on structural, thermal and optical properties. The manganese chloride doped itaconic acid single crystals (MCIA) were grown from aqueous solution by the slow evaporation method. The investigation has been made by subjecting the title compound to various instrument techniques. The lattice parameters obtained from a single crystal differ from the parent crystal and confirm the formation of the titled crystal. The purity of the grown crystal is proven from powder X-ray diffraction analysis. The FTIR analysis confirms the functional groups present. The variation of hardness number with load indicates the hard nature of the material. The UV-vis-NIR transmission studies show optical transparency in the entire visible region and has cut off length of 310 nm. From TGA/DTA investigations, it is observed that the manganese chloride doped itaconic acid crystals have thermal stability up to 160° C. The third order nonlinear optical nature of MCIA single crystals was studied using Z – scan technique.

Keywords: Crystal growth, optical Parameters, TG-DTA, third order NLO.

**"Biodegradable Nanomaterials: Revolutionizing the Food Industry – A
Comprehensive Review"**

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ABSTRACT

Nanomaterials have gained attention for their remarkable mechanical, thermal, optical, and antimicrobial properties due to their small particle size, extensive surface area, and high reactivity. Recently, these nanostructured materials have found applications in the food industry, addressing the challenges in food storage and preservation. Ensuring food safety has become increasingly critical as contaminated and expired food items lead to rising infections and fatalities. The food industry demands innovative solutions for quality control and safety measures.

Innovations in nano-food, nano-sensors, and nano-packaging have emerged as significant advancements. Nanomaterials offer unique attributes such as antimicrobial properties, biotherapeutic capabilities, extended shelf life, and preservation of food quality and flavor. Sugarcane bagasse, a fibrous residue from sugarcane juice extraction, can be repurposed to produce cellulose nano crystals, finding diverse applications. Nanotechnology in the food industry provides benefits in preservation, processing, and packaging. Nanosensors play a crucial role in detecting harmful components in food, while nanomaterials offer antioxidant features in food packaging, replacing petroleum-based plastics. Carbon materials, synthesized through eco-friendly methods, are gaining prominence as contamination-free alternatives for food packaging.

Additionally, nanosensors, including quantum dots, carbon nanotubes, and gold nanoparticles, have been designed to detect chemicals and toxins in food. However, careful selection of non-hazardous nanomaterials is essential to prevent adverse effects on both the environment and human health. Nanotoxicology, concerning the impact of

nanomaterials on food and health, remains a significant concern. The use of nanotechnology seems very much promising in the domain of Food industry and could have a great future in this regard. In this review, we discuss the applications of various organic-based nanomaterials being employed in the food industry, serving as carriers, biotherapeutic agents and enhancing food packaging, shedding light on their potential benefits and challenges.

Keywords: Nano materials, Food storage, Carbon nanotubes, Food packaging, nanosensor, nanotoxicology, Organic nanomaterials.

Structural and Luminescence Studies of BaB₄O₇:Eu Glass for Opto-Electronic Application.

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ABSTRACT

Borate glass with BaB₄O₇:Eu composition and Eu₂O₃ with 1.0 mol.% relative to B₂O₃ have been prepared by melt quenching method, and studied by X-ray diffraction (XRD), Fourier transform- infrared spectroscopy, optical absorption, EPR and luminescence spectroscopy. The EPR spectroscopy clearly show that the Eu is incorporated into the network of prepared glass. The basic structural trigonal (BO₃) and tetrahedral (BO₄) units in the glass were identified using Fourier transform infrared spectroscopic analysis. The linear optical properties such as refractive index and optical band gap energy of the Eu³⁺ ions doped barium borate were studied using UV-Visible spectroscopic analysis. The emission spectrum reveals five intense emission bands between 570-710 nm, with predominate peak at 615nm corresponds to ⁵D₀→⁷F₂ transition. The decay time, Judd-Ofelt parameters such as transition probabilities, branching ratio and radiative lifetime were estimated by using luminescence spectra. The higher Ω₂ parameter value specify the higher covalent nature and higher asymmetry around the Eu³⁺ ions in the glass. The CIE chromaticity coordinates of prepared sample was studied and found to x = 0.6604 and y = 0.3114 which belongs to red domain. The computed CCT value of Eu³⁺ ions doped Barium Borate glass was found to be 4384 K. The experimental results confirms that the prepared sample could be suitable for red LEDs and visible red lasers application.

Gas Sensor using Spectroscopy to Inhibit Fruit Ripening

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ABSTRACT

Fruits are essential elements of our diet, providing crucial nutrients and enhancing our culinary experiences with their flavors. Ripening is the natural process through which fruits and vegetables develop their desired taste, quality, color, and texture. While this process is natural, controlling it is vital to ensure that fruits are delivered to consumers in their best condition. Fruit ripening significantly impacts the agricultural industry, influencing the quality, shelf life, and marketability of fruits. This poses challenges for farmers, distributors, and retailers, leading to economic losses and increased food waste due to the shortened shelf life of fruits. Consequently, finding effective methods to control and delay fruit ripening has become a priority for the agricultural and food sectors.

Ethylene (C₂H₄), a natural plant hormone, is commonly used to induce fruit ripening before fruits enter the market. Monitoring ethylene levels precisely and continuously is crucial, as low ethylene concentrations produced by the fruit itself indicate its ripeness, while ethylene is sometimes externally added to promote ripening. To address this challenge, a gas sensor incorporating spectroscopy techniques has been developed to detect and regulate ethylene gas levels in fruit storage environments. Spectroscopy analyzes the spectral signatures of gases in the surroundings, allowing continuous monitoring of gas concentrations and spectral features. By observing the progression of fruit ripening, this system ensures accurate ethylene gas level control, preventing both over-ripening and under-ripening.

The gas sensor relies on the natural color changes of fruits and vegetables to indicate their ripening stages, correlating these stages with the required ethylene gas levels

for the ripening process. Fruits like apples, pears, bananas, and mangoes release ethylene during ripening, influencing texture, softness, color, and other ripening-related processes. Using spectroscopy principles, especially infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopy, the gas sensor accurately measures ethylene concentrations. By analyzing the specific spectral features of ethylene gas, the sensor offers real-time data on gas levels within storage facilities, indicating the level of fruit ripening. This measurement is essential during post-harvest and transportation to prevent over-ripening and ensure fruits reach consumers in optimal condition.

In conclusion, the gas sensor employing spectroscopy to prevent fruit ripening presents a promising solution for the agricultural industry's challenges. Its ability to detect and manage ethylene gas concentrations in real-time can revolutionize fruit preservation techniques, ensuring consumers have access to fresh, high-quality fruits while minimizing food waste.

Keywords: Ripening, Ethylene, spectroscopy, infrared (IR) and ultraviolet-visible (UV-Vis) spectroscopy.

**Characterization and Discriminenece of Different Types of Medical Imaging
Models in Image Processing**

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ABSTRACT

Medical imaging is the procedure used to attain images of the body parts for medical uses in order to identify or study diseases. There are millions of imaging procedures done every week worldwide. Medical imaging is developing rapidly dueto developments in image processing techniques including image recognition, anal-analysis, and enhancement. Image processing increases the percentage and amount of detected tissues. This chapter presents the application of both simple and sophistic-cated image analysis techniques in the medical imaging field. This Paper also summarizes how to exemplify image interpretation challenges using differentimage processing algorithms such as k-means, ROI-based segmentation, and water-shed techniques.

Keywords: Medical, Imaging, Image Processing Technique

Photocatalytic Activity of Zinc Oxide Doped Bismuth oxide Nanoparticles using Oxalic Acid as Reducing Agent

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ABSTRACT

The α -Bi₂O₃NPs were synthesized by precipitation method using oxalic acid as a reducing agent. The synthesized samples were characterized using X-ray diffraction (XRD), Fourier transform infrared spectrophotometer (FTIR), UV-DRS technique, Photoluminescence (PL), High Resolution Transmission electron microscopy (HR-TEM) and photocatalytic study. The XRD pattern revealed the crystalline phase of the Bi₂O₃NPs belong to α -phase with monoclinic structure. The FT-IR spectrum confirmed the presence of Bi-O bond. The UV-DRS spectrum indicated that the absorption edge is blue shifted and the bandgap of the synthesized sample was 2.80 eV. The HR-TEM revealed the presence of spherical, cylindrical and some irregular particles. PL study provided the information about electronic band transitions, and structure as well as defects. The photocatalytic activity of the samples were studied in the degradation of Methylene blue (MB) and Crystal Violet (CV) under visible light irradiation. The pure α -Bi₂O₃NPs showed the highest degradation after 135 min of irradiation.

Keywords: ZnO, α -Bi₂O₃, Methylene Blue, Crystal Violet and Photocatalytic activity

**Bio - Synthesis and Characterization of ZnONps Using
*AndrographisPanicuata*leaf Extract**

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ABSTRACT

The present work focuses on the green synthesis of Zinc Oxide nanoparticles using aqueous solution of *AndrographisPanicuata*leafextract. Zinc Oxide is used as precursor for the preparation and *AndrographisPanicuata*leafextract is used as an effective reducing agent. The optical properties of biosynthesized ZnO nanoparticles are characterized by the UV-Vis spectrum recorded the maximum absorbance peak at 355 nm and the obtained value of optical band gap is 3.12 eV (Tauc's equation). The Fourier transform infrared, FTIR, spectra of the plant extract and ZnO NPs were examined to figure out if the functional groups related to these reductive biomolecules exists and specifying the functional groups that contributed to reduction of the ZnO into nanoparticles *AndrographisPanicuata* Leaf extract. The results of X-ray diffraction (XRD) the exhibited peaks correspond to the (100), (002), (101), (102), (110), (103), and (112) of a hexagonal wurtzite structure of ZnO is identified using the standard data, The calculated values of the lattice constants of ZnO-NPs are $a = 3.2473 \text{ \AA}$ and $c = 5.1917 \text{ \AA}$ (size 24 nm). The study of SEM images shows that as-prepared ZnO nanoparticles are spherical and fluorite in shape with slight agglomeration and EDAX spectroscopy confirms the presence of Zn and O in the samples with high purity. Thermal analysis (TGA/DTA) the total weight-loss 20% and breakdown of organic groups existing in the specimen through the biosynthesis process, the endothermic and exothermic peak observed in the DTA curve. The antibacterial activity was studied with gram-negative and gram-positive bacteria such as *Bacillus cereus*, *E.coli* was considered statistically significant, and Antifungal activity was *Aspergillusniger* Zone of inhibition in mm was carried out.

Keywords: Zinc Oxide nanoparticles, UV-Vis, FTIR, XRD, SEM/EDAX, TGA/DTA, Antibacterial and Antifungal activity's.

**Optical, Structural, Mechanical, Electrical, Magnetic and Electrochemical
Properties of Barium Strontium Manganese Borate Glass.**

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ABSTRACT

The barium strontium manganese (BSM) borate glass was produced by quenching method. The optical band gap of BSM borate glass estimated through Uv-Vis-NIR spectroscopic analysis was found to be 3.9 eV. The dielectric constant, $\tan \delta$ and electrical conductivity were studied for the prepared sample using LCR meter at room temperature. The mechanical behaviours of BSM borate glass was calculated by Vickers hardness tester. The surface of BSM borate glass was identified using SEM analysis. The magnetic property of the BSM borate glass was analysed using VSM. The electrochemical properties of BSM borate glass electrodes were investigated using cyclic voltammetry (CV) analysis. The specific capacitance and capacity retention of BSM borate glass was calculated from the above studies and the results are discussed in this paper.

Keywords: Borate glass, Cyclic Voltammeter, Vickers hardness number, Dielectric measurement.

TRAFFIC DETECTION IN WIRELESS SENSOR NETWORKS

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ABSTRACT

During the last few decades, the sensor based Ad-hoc network known as Wireless Sensor Networks has become popular in various fields. This special purpose networks are introduced to solve the many real world problems inexpensively and easily too. These Wireless Sensor Networks are composed of thousands of interconnected low cost nodes. Each and every node has limited communication power with some sensing capabilities and even less computation. The sensor nodes gather the essential information from the area which is being monitored. The collected data is then forwarded via intermediate sensor nodes (relay) to the Base Station. Once the network is deployed, the deployed environment of Wireless Sensor Networks is non-central, unattended and administrative less. Therefore malicious attack such as Distributed Denial of Service attacks which is a common attack can easily be commenced by the attackers. In this attack, the attacker tries to stop the victim's ability to use its bandwidth or respond to any request. This attack is obtained by transmitting the bulky requests to the victim in a very short period of time. The victim node becomes incapable of responding or processing the requests, on receiving such requests in bulk. While having such scenario, the entire networks performance is affected extremely. Most of the distributed denials of service detection system rely on the analysis of the flow of traffic, eventually with a conclusion that high traffic may be due to the distributed denial of service attack. The challenge here is to detect the abnormal traffic. To overcome this, a new model is planned to be proposed.

Keywords: WSN; DDoS Attack; Abnormal Traffic.

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Influence of Ce³⁺ (Rare Earth Element) on the Structural, Morphological, Impedance, Binding energy and Ferrimagnetic properties of Spinel ZnFe₂O₄ Nanoparticles fabricated by the Co-precipitation method with varying annealing temperature: Antibacterial activity

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ABSTRACT

A large ionic radii cerium (REE) ion was compactly coupled to zinc ferrite (ZnFe₂O₄) using a simple co-precipitation method with varying annealing temperature. Cerium ion greatly modifies the structure, magnetic properties and microcolony of ferrites. A change in crystallite size and lattice constant can be observed as temperature changes. XRD reveals that the crystallite size changes with temperature. The FT-IR resonance spectra reveal that the spinel ferrite structure is possible due to oxygen co-vibration with Ce³⁺ and Fe³⁺ ions in tetrahedral and octahedral voids. HR-TEM revealed high crystallinity of the ferrite matrix and magnetic domain formation. The chemical state of all metal ions in the ferrite alloy was confirmed by XPS. The impedance analysis clearly shows that all the doped samples have higher electrical conductivity. VSM clearly shows that cerium (REE) ion affects the magnetic factors of coercivity (H_c), remanent magnetization (M_r), saturation magnetization (M_s) and confirms the presence of ferriparamagnetic materials. As the remanent ratio is found to be less than one (> 1) soft ferrite is acquired. Antibacterial activity analysis showed that the magnetic nanoparticles were effective in killing bacteria. This type of nanoparticles penetrated the cell walls of Gram positive bacteria (G⁺) and Gram negative bacteria (G⁻) and stabilized the microbial colony.

Keywords: zinc ferrite, co-precipitation, ferriparamagnetic, Antibacterial activity, cerium

**Optical Analysis of Nickel Doped Zinc Sulfide Nanomaterials by Sol - Gel
Method**

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ABSTRACT

Nanomaterials synthesis and its application have increased vastly in the last two decades. There are various methods of synthesis and processing employed in industries to exploit to their production values in its cheapest way. Zinc sulfide is a prominent member of II-IV semiconductor with a various applicable properties. Addition of dopant will make such transition metals to have enhanced Optical Property. In the meanwhile, the synthetic ways also act on the properties of nanomaterials. In this paper, Nickel doped Zinc Sulfide nanomaterials were synthesized using Sol-Gel method. The synthesized nanomaterials were subjected to different Characterizations like X-ray diffraction (XRD), UV-Visible Spectroscopic (UV-VIS) study and Photoluminescence study (PL). The Structural Analysis reveals the Cubic Structure of the as synthesized Nickel doped Zinc Sulfide nanomaterials. From UV-VIS spectroscopy, the cut off wavelength and hence its energy band gap is determined. It shows Good Optical Transparency in entire visible region and near UV region. The different excitation wavelengths and emission wavelengths from the synthesized Nickel doped Zinc Sulfide nanomaterials are observed from PL. The peak position of PL spectra shows huge red shift in the emission peaks and finds its applications in the making of LEDs.

Keywords: ZnS, Optical Property, UV-Visible, PL Spectra.

**Preparation and Characterizations of Undoped and Doped Bismuth Oxide
Nanoparticles Using Precipitation Method**

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ABSTRACT

CuO-doped of Bi₂O₃ and undoped Bi₂O₃ nanoparticles were prepared using nitric acid assisted co-precipitation method with different concentrations. The prepared powders annealed at 700°C were characterized using powder X-ray diffraction (XRD), Thermo gravimetric / Differential Thermal Analyzer (TG-DTA), Fourier transform infrared spectroscopy (FTIR) and UV-Visible spectroscopy (UV-Vis), photoluminescence (PL) and High Resolution scanning electron microscopy (HR-SEM). The XRD pattern of the prepared samples revealed the monoclinic structure of Bi₂O₃. The band gap value calculated from UV-DRS spectra shows a variation in the range 2.3 to 3.0 eV. The presence of metal oxide bands in FTIR was confirmed from peak in the region 400-700 cm⁻¹. A noticeable change in morphology is observed in HR-TEM.

Keywords: Nano Composites; Cell volume; particles size; band energy gap; functional group

Characterization and Luminescence Properties of BaMgSi₂O₆:Eu²⁺ Phosphor

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Oxides and silicates based materials possess better chemical stability compared to fluoride and sulfide based host lattice. The silicate lattices have proved themselves as capable host to be doped with lanthanide ions due to brilliant optical properties in visible range. Rare earth silicate based phosphors, have attracted interest of researchers due to their high efficiency as a host, excellent thermal and chemical stability and high brightness adding to their low cost [1]. These phosphors showed great potential in various applications such as fluorescent lamps, white light emitting diodes, and display components. High temperature solid-state reactions are usually employed to synthesize the compounds [2]. BaMgSi₂O₆:Eu²⁺ blue phosphor was prepared by the solid-state reaction method and the phosphor characterized in terms of crystal structure, particle size, photoluminescence (PL), thermoluminescence (TL), X-ray diffraction (XRD), Scanning electron microscopy (SEM). The XRD result shows that phosphor is formed in a single phase and has a monoclinic structure. Furthermore, the PL excitation spectra of Eu²⁺ doped BaMgSi₂O₆ phosphor showed a strong band peak at 356 nm and the PL emission spectrum has a peak at 520 nm.

Keywords: BaMgSi₂O₆, Europium Oxide, Silicate phosphor, Photoluminescence

**Energy Efficient Data Transmission to Enhance Network Lifetime of Wireless
Sensor Networks**

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ABSTRACT

Wireless Sensor Networks are composed of a large number of inexpensive micro sensor nodes deployed in the monitoring area. One of the major challenges in WSN is energy efficient data transmission due to its battery-powered sensor nodes. Wireless Sensor Networks have a great attention due to its vast range of applications including natural disaster prevention, healthcare monitoring, smart home development and water quality management. WSNs consist of sensor nodes that monitor physical events such as humidity, pressure, temperature, light and vibration over a geographic area. WSNs enable new applications and require non-conventional paradigms for protocol design due to several constraints. Owing to the requirements for low device complexity with low energy consumption (i.e. Long network lifetime), a proper balance between communication and signal/data processing capabilities motivates to do research in Wireless Sensor Networks. Further, the communication range of sensor nodes is limited and therefore, multi-hop communication is the only option for forwarding data to base station (BSs). However there are several disadvantages in multi-hop communication such as unavailability of a suitable active relay, low battery energy of the relays and frequent disconnection of links due to channel variability. Routing in WSN is also an important aspect where energy efficiency, network lifetime and quality of Service (QoS) are required to be considered along with its unique structural characteristics. Hence it is planned to propose energy efficient algorithms to enhance the lifetime of sensor nodes and Wireless Sensor Networks.

Keywords: WSN; Data Transmission, QoS; Lifetime Enhancement.

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**Energy Efficient Algorithms with Minimal Detection Time for Rare Event
Detection in Wireless Sensor Networks**

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ABSTRACT

Wireless Sensor Networks play a major role in revolutionizing the world by its sensing technology. It is used to monitor physical or environmental conditions, such as temperature, sound and pressure. There are several design challenges pertaining with WSN such as scalability, localization, routing, energy consumption, security and storage capacity etc. Energy saving in wireless sensor networks have attracted a lot of attention in the recent years. It is one of the critical aspects for WSNs. WSN has emerged as a powerful technology which has multiple applications such as military operations (battle field surveillance), industrial applications (industrial process monitoring) and consumer applications (health monitoring), surveillance system, Intelligent Transport Systems (ITS) etc. Rare Events Detection is one of the important application of WSN. Rare Event is an event is considered unusual when it occurs despite having a low likelihood of happening such as Volcanic Eruptions, Forest fire and Land slide etc.

Rare event has a low probability of happening and are unpredictable, so it is challenging to ensure that duty cycled battery-powered sensing nodes will be activated when rare events take place. Nodes in wireless sensor networks (WSNs) often operate in low duty cycle mode to conserve energy, which results in a considerable delay in event detection and data transfer to the sink and impairs the network's effective processing of the event. There exists a trade-off between rare event detection delay and network lifetime. The most energy efficiency is possible with low duty cycle operation, when a node conserves energy by operating in a low power state and is active for a short amount of time. It is planned to design algorithms to enhance lifetime of sensor nodes with minimal detection delay and low duty cycling for rare event detection.

Keywords: WSN, Rare Event Detection, Network Lifetime, Duty Cycle.

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Wireless Water Communication and GPS Based Fisherman Tracking

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ABSTRACT

The most difficult medium for data communication is the underwater medium. It is due to its characteristics. The various existing modes of communication in water mediums are acoustic waves and optical signals. To overcome these, in our proposal, an EM technique is used for data transmission in a water medium. It uses Magnetic Transmitter sources for transmission of data. This will ensure the maximum transmission rate and it is more efficient and cheaper than the other existing methods. In our proposal, automation via GPS tracking capabilities is also incorporated. Our proposed system has the aim to give a well-understandable user-friendly technological mobile computing gadget. To support and give enough awareness of IMBL (International Maritime Boundary Line) and protect them not to cross the maritime boundary at any cost. And give full secureness and reliable safety for Indian fishermen's lives. To perform this task some modern concepts of mobile computing methods have to be taken into hands. In this project, we are using LoRa (Long Range) wireless communication technology. WWSNs (Wireless Water Sensor Network), which have components, i.e., the sensors, that are buried underwater and that communicate through Water. The majority of the applications for WWSNs –are intelligent communication, and environmental monitoring, of the Water. In this proposed system emergency messages are received and sent to the centralized server or fishermen's boat through water for emergency conditions.

Keywords: GPS; LoRa; IMBL; WWSNs

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Hydrothermal Synthesis of $Zn_2SiO_4:Mn$: Structural, Morphological, and Luminescence Property Analysis.

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ABSTRACT

Nano-sized $Zn_2SiO_4:Mn$ phosphor were synthesized by hydrothermal method using cetyltrimethylammonium bromide (CTAB) surfactant. The phosphors were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and photoluminescence (PL). The average particle size calculated by Debye Scherer's equation is 30 nm. Synthesized $Zn_2SiO_4:Mn^{2+}$ exhibited green emission at 525 nm, which was attributed to the ${}^4T_1-{}^6A_1$ transition of Mn^{2+} excited at 254 nm. The SEM study revealed $Zn_2SiO_4:Mn$ synthesized by hydro-thermal techniques formation of spherical nanoparticles with size 10–25 nm. The PL emission intensities of micron-sized $Zn_2SiO_4:Mn^{2+}$ phosphors synthesized by solid-state reaction and pyrolysis are more intense with better CIE coordinates and compared with nano-sized $Zn_2SiO_4:Mn^{2+}$ synthesized by hydrothermal technique. The morphology of CTAB-assisted phosphor is, however, better than other techniques and commercial ones.

Keywords: Nano phosphors, green phosphors, $Zn_2SiO_4:Mn^{2+}$ phosphor

Synthesis and Luminescence Properties of BaSO₄:Eu²⁺

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ABSTRACT

Eu doped BaSO₄ was prepared by the recrystallization method and characterization of the material was done by using X-ray diffraction (XRD), scanning electronmicroscope (SEM), energy dispersive spectroscopy (EDS) and Fourier transform infrared spectroscopy (FTIR) techniques. From the XRD pattern of Eu doped BaSO₄ compound, it was found that the prominent phase formed was BaSO₄ and traces of other phases were very weak. The room-temperature PL spectra of the Eu doped BaSO₄ sample showed one peak centered at 374 nm, which is the characteristic emission of Eu²⁺ ion. This emission band at 374 nm corresponds to the 4f⁶ 5d → 4f⁷ (⁸S_{7/2}) transitions of Eu²⁺ ions. The excitation spectrum taken at the wavelength 375 nm extends over a wide range of wavelengths from 220–350 nm with a strong peak at around 310 nm. Furthermore, the present sample shows good crystal quality and high photoluminescence sensitivity.

Keywords: BaSO₄,Europium Oxide, Sulphate phosphor, Photoluminescence,

Characterization and Luminescence Properties of SrSO₄:Eu²⁺ Phosphor

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ABSTRACT

Rare-earth activated SrSO₄ has found wide applications in radiation dosimetry with the merit of high sensitivity to low-level radioactivity. The rare earth ions in SrSO₄, such as Tb³⁺, Eu²⁺ and Dy³⁺, work as luminescence centers to give off efficient emissions under the X-ray and gamma ray irradiations. Apart from working as thermoluminescent materials, SrSO₄, which is a typical insulator with a wide bandgap of about 7.6 eV, can also be utilized as the host of rare-earth dopants for the development of efficient phosphors under ultraviolet (UV) excitation. Indeed, several groups reported the photoluminescence (PL) of rare-earth doped SrSO₄ upon UV excitation. For example, Di et al. reported the violet-blue PL of Eu²⁺ doped SrSO₄ under the excitation of 260 nm, Gong et al, separately recorded the PL of Eu²⁺ and Eu³⁺ doped SrSO₄ under the excitation of 246 nm, Sun et al, explored the orange PL of Sm³⁺ doped SrSO₄ under the excitation of 401 nm, and Yamashita et al, observed the green PL of Tb³⁺ doped SrSO₄ under the excitation of 352 nm. These results have unveiled the potential of rare-earth doped SrSO₄ as efficient phosphors for LED and other information display devices.

Keywords: SrSO₄,Europium Oxide, Sulphate, Photoluminescence

Characterization and Luminescence Properties of BaMgSi₂O₆:Eu²⁺ Phosphor

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ABSTRACT

Oxides and silicates based materials possess better chemically stability compared to fluoride and sulfide based host lattice. The silicate lattices have proved themselves as capable host to be doped with lanthanide ions due to brilliant optical properties in visible range. Rare earth silicate based phosphors, have attracted interest of researchers due to their high efficiency as a host, excellent thermal and chemical stability and high brightness adding to their low cost [1]. These phosphors showed great potential in various applications such as fluorescent lamps, white light emitting diodes, and display components. High temperature solid-state reactions are usually employed to synthesize the compounds [2]. BaMgSi₂O₆:Eu²⁺ blue phosphor was prepared by the solid-state reaction method and the phosphor characterized in terms of crystal structure, particle size, photoluminescence (PL), thermoluminescence (TL), X-ray diffraction (XRD), Scanning electron microscopy (SEM). The XRD result shows that phosphor is formed in a single phase and has a monoclinic structure. Furthermore, the PL excitation spectra of Eu²⁺ doped BaMgSi₂O₆ phosphor showed a strong band peak at 356 nm and the PL emission spectrum has a peak at 520 nm.

Keywords: BaMgSi₂O₆,Europium Oxide, Silicate phosphor, Photoluminescence,

Luminescence and Optical Properties of SrMgSi₂O₆:Eu²⁺ Phosphor

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ABSTRACT

Rare earth ions doped phosphors have been used in varied fields based on their electronic and optical characters arising from their 4f electrons. Among the rare earth elements, europium is a special element as dopant, because it exhibits the property of valence fluctuation, i.e., the valence state is divalent or trivalent and it shows different characteristics luminescence due to the different valence [1]. Recently strontium magnesium silicate phosphor has attracted great interest due to its special structure features, excellent physical and chemical stability. Alkaline earth silicate is an important luminescent material because of its excellent chemical, thermal stabilization and cheap raw material SiO₂ [2]. We synthesized SrMgSi₂O₆:Eu²⁺ phosphor by solid state reaction method and studied the luminescent properties. Investigations on the crystal structure of sintered phosphors were determined by the X-ray diffraction (XRD). Luminescence properties were also investigated on the basis of photoluminescence (PL) and thermoluminescence (TL). The PL excitation spectra of Eu²⁺ doped SrMgSi₂O₆ phosphor showed a strong band peak at 356 nm and the PL emission spectrum has a peak at 440 nm.

Keywords: SrMgSi₂O₆,Europium Oxide, Silicate phosphor, Photoluminescence,

Synthesis and Photoluminescence properties of (Ba,Sr)SO₄:Eu²⁺ Phosphor

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ABSTRACT

The rare earth doped luminescent materials play integral role in modern life with tremendous applications ranging from color display, Scintillators, fluorescent lamps, intensifying screens, dosimetry of ionizing radiations and so on [1]. The optical properties of phosphor materials are influenced by chemical composition and by the presence of dopants or impurities and its concentration. Metathesis (double exchange) reaction taking place in solid state are not quite common. However, these extremely fast, self-energetic reactions yield crystalline materials in very short time intervals with unusual microstructures [2]. We synthesis (Ba,Sr)SO₄:Eu²⁺ using solid state synthesis. In solid state metathesis, exchange of bonds between the two reacting chemical takes place and results in creation of products having identical bonding affiliations. Investigations on the crystal structure of sintered phosphors were determined by the X-ray diffraction (XRD). Luminescence properties were also investigated on the basis of photoluminescence (PL) and thermoluminescence (TL). PL studies exhibit the emissions at 375 nm and excitation at 290 nm respectively.

Keywords: (Ba, Sr)SO₄,Europium Oxide, Sulfates, Photoluminescence,

Synthesis and Photoluminescence properties of $\text{CaMgSi}_2\text{O}_6:\text{Eu}^{2+}$ Blue Phosphor

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ABSTRACT

Rare earth silicate based phosphors, have attracted interest of researchers due to their high efficiency as a host, excellent thermal and chemical stability and high brightness adding to their low cost. These phosphors showed great potential in various applications such as fluorescent lamps, white light emitting diodes, and display components. High temperature solid-state reactions are usually employed to synthesize the compounds. $\text{CaMgSi}_2\text{O}_6$ is one of the pyroxene minerals consisting of single SiO_4 tetrahedra connecting with each other along one of the axis in the unit cell [1]. Generally, rare earth ions doped CMS phosphors are synthesized from usual solid-state method at higher temperatures [2]. In this work, $\text{CaMgSi}_2\text{O}_6:\text{Eu}^{2+}$ have been prepared by solid-state synthesis and the optical characteristics and fluorescence were studied. Phase identification by XRD and the measurements of photoluminescence (PL) excitation and emission spectra were recorded. XRD results showed that the pattern of the prepared phosphors were well matches with JCPDS file No. 19 - 0239. PL studies exhibit the emissions at 450 nm and excitation at 340 nm respectively.

Keywords: $\text{CaMgSi}_2\text{O}_6$, Silicate phosphor, Photoluminescence, Solid-State Synthesis

The Current State of Image Processing And Big Data Analytics: Issues and Challenges

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ABSTRACT

This Presentation explores the fascinating world of Digital Image Processing, a dynamic field at the intersection of Computer Science and visual perception. In today's data driven world, the ability to manipulate and analyze images holds immense significance. This will provide an overview of the fundamental concepts, techniques and recent advances in digital image processing.

Basic image understanding as data and the function of digital processing are evident in the Introduction. The Fundamental Steps Image Enhancement, Image Segmentation, Object Recognition and Classification, Image Restoration and Image Compression. The Problems are Noise and Distortion, Object detection and Recognition, Data Annotation and Labeling and Computational Resource Intensity. They particularly use noise reduction techniques and algorithms such as non-local means, wavelet denoising method. The Processing starts with detecting objects using a computer vision technique. The real-world applications of digital image processing in fields such as medicine, astronomy and computer vision. This provides an comprehensive overview of digital image processing, showcasing its practical significance in various domains and inspiring further exploration of this exciting field.

Keywords: Digital Image Processing; Noise Distortion; Wavelet Denoising.

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Different Metal Doped ZnO Nanoparticles for Sunlight Mediated Degradation of Polypropylene Films

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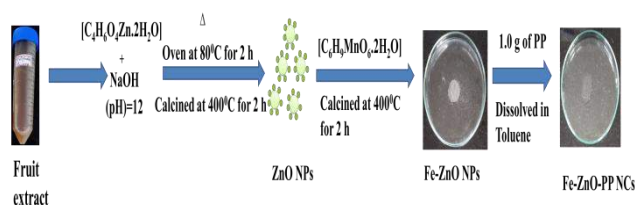
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ABSTRACT

Different metal-doped zinc oxide nanoparticles (DMD-ZnO NPs) were synthesised using fruit extraction, and a fruit-assisted green technique was used to degrade polypropylene (PP) plastic when exposed to sunlight. The optical and structural properties of green synthesised materials were investigated using UV–vis spectroscopy, Fourier transform infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM) with energy dispersive x-ray (EDX) analysis, X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD) techniques. According to the weight loss data, the photocatalytic activity of the DMD-ZnO-PP film was greater than that of pure PP and un-doped ZnO-PP films. Because of their increased optical absorption and efficient suppression of photo-produced charge carriers, the DMD-ZnO NPs showed stronger photocatalytic degradation of PP. The formation of carbonyl groups (C=O) as the degradation product of PP was confirmed by Fourier transform infrared (FT-IR) analysis. Thus, PP films with 2% wt Fe-ZnO film nanomaterials showed a degradation of around 37% among DMD-ZnO-PP nanocomposites (NCs) films under visible light over a short period of 30 days (240 h). The study therefore suggests the incorporation of DMD-ZnO NPs into the polymer matrix so as to enhance its photodegradation.



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An Overview of Deep Learning-Based Wireless Communication Technologies

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ABSTRACT

The field of wireless communications has undergone a remarkable transformation in recent years, driven by technological innovations and an ever-increasing demand for high-speed, reliable connectivity. This comprehensive presentation explores the latest advancements in wireless communication technologies, protocols, and applications.

Furthermore, this abstract highlights the key challenges in wireless communications, including spectrum scarcity, security concerns, and latency requirements, and discusses potential solutions and future directions in these areas. We also examine the proliferation of Internet of Things (IoT) devices and their impact on wireless networks. Then, We can see the Cellular Systems, Wireless Lans, Satellite Systems and PANS. With the development of 5G, the future wireless communication network tends to be more and more intelligent. Ultimately, this presentation provides an overview of wireless communications, offering a foundation of wireless technology and address the connectivity needs of our increasingly connected world.

Keywords: Artificial intelligence; Wireless communication; Cellular Systems;

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**Modified 10T Tunnel Field Effect Transistor SRAM Cell with Low Power and
Improved Noise Margin**

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ABSTRACT

Tunnel field-effect transistors (TFETs) have been proposed as an alternative to conventional MOSFETs for ultra-low voltage operation. The TFET devices' inherent steep Subthreshold Slope properties enable low voltage operation while minimizing leakage-dominated power dissipation. However, the static random-access memory (SRAM) circuit's performance can be significantly worsened by the forward p-i-n current of the TFET. 10T TFET SRAM cell with cascode isolation transistors that is half-select disturb-free is proposed. In this work, we suggest a 10T TFET SRAM cell that has a separate read port to improve the read static noise margin (RSNM) and the write static noise margin (WSNM). The drain of the read access transistor (N-type TFET) is always higher than the source and the source of the write access transistor (P-type TFET) is always higher than the drain. This prevents the application of forward bias to the p-i-n junction thus eliminating the impact of the forward p-i-n current. As a result, the static noise margin (SNM) of SRAM cells is improved, and write and leakage power consumption are both significantly reduced.

Keywords: Tunnel Field-Effect Transistors (TFETs), SRAM, ultra-low power, forward p-i-n current, SRAM, read static noise margin (RSNM), write static noise margin (WSNM)

**Density Functional Theory studies – A boon to Vibrational Spectroscopic
research**

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ABSTRACT

Vibrational spectroscopy is a valuable tool for the elucidation of molecular structure. Vibrational spectra can be utilized directly and simply as molecular fingerprints to characterize and identify a molecule. Recent developments in Fourier Transform Spectrometers have led to higher resolution, total wavelength coverage, higher accuracy in frequency and intensity measurements. Moreover, sophisticated computational methods of theoretical chemistry have also been developed by powerful personal computers. This has made it possible to perform a complete vibrational analysis on relatively large polyatomic molecules. The utilization of vibrational spectroscopy as an effective tool in the elucidation of molecular structure has now become more with the introduction of Fourier transform infrared spectrometers and lasers as source for recording Raman spectra. Vibrational spectroscopy has contributed significantly to the growth of different areas as polymer chemistry, catalysis, fast reaction dynamics, charge – transfer complexes etc.

For a proper understanding of IR and Raman spectra, a reliable assignment of all vibrational bands is essential. For this purpose, quantum chemical methods are invaluable tools. Among them, Density Functional theory (DFT) methods have evolved as powerful quantum chemical tool for the determination of the structure of molecules. In the frame work of DFT approach, different exchange and correlation functionals are routinely used. Among these, the B3LYP combination is the most used since it proved its ability in reproducing various molecular properties, including vibrational spectra. Further, it gives the information about the interactions both in filled and virtual orbital spaces which could enhance the analysis of intra and intermolecular interactions.

Detection of Corona Virus Using a Biosensor

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ABSTRACT

Metamaterials research has emerged in a number of sectors over the past two decades. Metamaterials are materials that have been created artificially and contain characteristics that are not found in natural materials. For biological sensors, the terahertz frequency range is frequently used. In order to find the SARS-CoV-2, we created an absorber in the terahertz frequency band. The sensitivity of the designed sensor is 12400 GHz/RIU.

Keywords: metamaterials, terahertz, sensitivity.

Detection of Cancer Cells Using Terahertz Metamaterial

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ABSTRACT

The terahertz gap is the region of the electromagnetic spectrum between microwave and far-infrared frequencies. The regime can be used for identification of the various elements in the sensing layer. In this work, we design a narrow-band absorber for a biological sensor. In particular, it can be useful in the biological sensor to distinguish between healthy and cancerous cells. The proposed sensor has a sensitivity of 916 GHz/RIU.

Keywords: Terahertz, absorber, biosensor, sensitivity.

Detection of Microorganisms Using Terahertz Range Metasurface Biosensor

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Abstract

Microorganisms, often referred to as microbes, are tiny living organisms that are too small to be seen with the naked eye. They include bacteria, viruses, fungi, protozoa, and some algae. Microorganisms play a crucial role in various ecosystems, from breaking down organic matter to aiding digestion in animals. Microorganisms are found almost everywhere on earth - air, soil, water, and even within other living organisms. So the detection of microorganisms is a major challenge in the medical and industrial sectors. So we have designed a biosensor for the detection of microorganisms in the environment. The terahertz frequency regions are widely used for biological sensors. Here, we have designed an absorber in the terahertz frequency range that can be used to detect microorganisms. The sensitivity of the proposed sensor is 390 GHz/RIU.

Keywords: terahertz, sensor, microorganisms.

**Synthesis and Characterization of Sn Doped ZnO Thin Films with Fabrication of
n-Sn: ZnO/P- Si/Ag P-N Junction Diode**

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ABSTRACT

A highly transparent and conducting p-Si and n-ZnO thin film was deposited by sol-gel spin coating method at 550°C for 1 hr. The XRD results confirm the wurtzite structure of ZnO films. The band gap energy for ZnO films was found to decrease with increasing Sn concentration. Surface morphology studies using FESEM revealed the smooth nature of the films and observed for pure and Sn doped ZnO films are slightly change in microstructure due to the main role of the pre-heated temperature during formation of thin films. 91 The all-solution grown p-n junction diode fabricated in the device structure n-Sn:ZnO/pSi/Ag showed a diode-like behavior with a knee voltage 2.0 V. The present study emphasize the applicability of all-solution grown p-Si/n-ZnO heterojunctions for the development of efficient and low cost optoelectronic devices particularly solar cells.

Keywords: ZnO, Solar cell, P-N junction diode, Band gap, Sol-gel

**Phase Stability, Optical and Dielectric Properties of Sm Doped ZrO₂
Nanoparticles Prepared by Co-Precipitation**

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ABSTRACT

Nanocrystalline samarium (1, 5 and 10 mol %) doped zirconium oxide (SZ1, SZ5, SZ10) are synthesized by simple co-precipitation technique and the calcination temperature was kept at 700°C for 2h to improve crystallinity. The crystal structural, optical and dielectric measurements were taken. The powder samples are in mixed phases of tetragonal and monoclinic crystal structures which was confirmed through X-ray Diffraction (XRD). The Raman spectra also confirmed that the presence of tetragonal and monoclinic phases. Bandgap values of the nanoparticles (5.24eV to 4.70eV) decreases with increasing the dopant concentration. Photoluminescence spectra revealed strong and broad emission at 375 nm in the UV region and 466, 505, 557 and 692 nm due to multiple emission (blue, green and red) in the visible region. The dielectric studies were performed for all the samples. The dielectric constant of ZrO₂ increased with Sm doping.

Keyword: XRD, UV-Vis, Photoluminescence, Dielectric Permittivity.

Synthesis and Electrochemical Characterization of MgMn_2O_4 Nanostructures for Supercapacitor Applications

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ABSTRACT

In this study, MgMn_2O_4 nanostructures were synthesized using a co-precipitation method involving KOH-NaOH. The crystal structure purity, functional groups, and morphology of MgMn_2O_4 were analyzed through X-ray diffraction (XRD), Fourier Transform Infrared Spectroscopy and scanning electron microscopy (FE-SEM). The electrochemical behavior of MgMn_2O_4 as an active material for supercapacitors was investigated. The electrode exhibited excellent capacitive behavior and superior electrochemical properties. The Nanostructure with ample free space proved beneficial in enhancing electrochemical performance. Specifically, the MgMn_2O_4 electrode demonstrated a faradaic capacitance, reaching a maximum specific capacitance of 355 Fg^{-1} at a scan rate of 5 mVs^{-1} . Furthermore, the electrode maintained a high coulombic efficiency of 100% even after 5000 charging-discharging cycles. The nanostructures of MgMn_2O_4 significantly contributed to the excellent electrochemical performance of the fabricated electrode. The results are discussed in detail.

Keywords: Co-precipitate; Pseudocapacitor; EDS; long-term stability; XRD; SEM

**Crystal Growth and Characterization of Piperazinium Ammonia chloride Hydrate
(PACH)**

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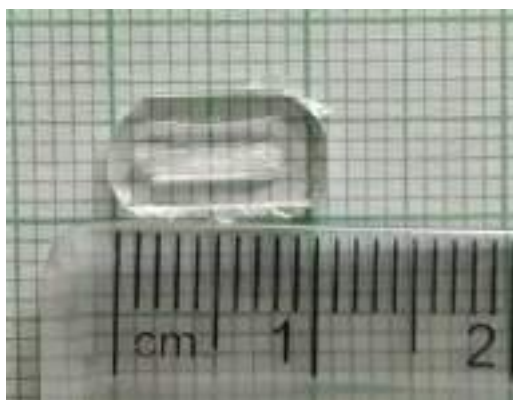
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ABSTRACT

Piperazinium Ammonium Chloride Hydrate (PACH) compound was successfully synthesized by using aqueous solution as solvent. The slow evaporation solution growth technique was used to grow a good optical quality single crystal of PACH at room temperature. The presence of distinct Bragg's peak in the powder X-ray diffraction analysis confirms the crystalline nature of the grown PACH sample. The thermal stability of the PACH single crystal has been investigated by Thermogravimetric and differential thermal analysis (TG-DTA). The as-grown PACH crystal's work hardening coefficient was calculated as $n=3.1$, indicating that it is a soft material. The dielectric constant and dielectric loss of the grown PACH crystal were analyzed as a function of different frequencies for different temperatures. The results are discussed in detail.



Photograph of as grown single crystal of PACH

Computational Approaches for Assessing the Anti-Influenza Potential of a Quinolone Derivative: A Synergy of Structure Optimization, Molecular Docking, and Pharmacokinetic Predictions

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ABSTRACT

Influenza, a highly contagious respiratory viral infection, continues to be a significant global health concern. With the emergence of drug-resistant strains and limitations of existing antiviral therapies, the quest for innovative and more potent treatments is paramount. This study explores the potential of 7-(benzo[d]oxazol-2-ylmethyl)quinolin-2(1H)-one as a promising anti-influenza drug candidate through a multifaceted approach, integrating structure optimization, molecular docking, and ADME (absorption, distribution, metabolism, excretion)/pharmacokinetic prediction techniques.

Employing a structure-based design methodology, computational strategies were employed to fine-tune the molecular configuration of the quinolone derivative, optimizing its capacity to interact with the viral target protein. Subsequently, molecular docking investigations were conducted to elucidate the binding interactions between the refined compound and the influenza virus protein, yielding insights into the binding mode, affinity, and key interacting residues. These findings provide a rational basis for the potential anti-influenza activity of the compound.

Additionally, ADME/pharmacokinetic prediction studies were executed to gauge the compound's drug-like properties, pharmacokinetic characteristics, and potential toxicity. These forecasts enabled the estimation of critical pharmacokinetic parameters encompassing absorption, distribution, metabolism, and excretion. This data is invaluable for gauging the compound's suitability for further development as an anti-influenza drug. In sum, this comprehensive computational investigation, amalgamating structure optimization, molecular docking, and pharmacokinetic predictions, illuminates the

promise of 7-(benzo[d]oxazol-2-ylmethyl)quinolin-2(1H)-one as an anti-influenza drug molecule. The insights gleaned from this research serve as a cornerstone for forthcoming experimental inquiries and underscore the pivotal role of computational methodologies in expediting drug discovery and development endeavours.

Keywords: Influenza, Anti-influenza drug, Quinolone derivative, Structure-based design, Molecular docking, ADME.

Synthesis, Growth and characterization of diaquabis [4-(2-aminoethyl) morpholine] nickel (II) dichloride single crystal

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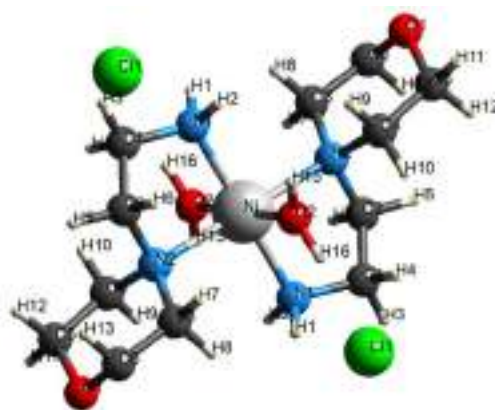
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ABSTRACT

The coordination of a morpholine molecule to a metal ion activates the morpholine molecule as a hydrogen bond donor by increasing the partial positive charge of the morpholine amine hydrogen. The transition metal ions as a source of magnetic moment and connect the metal ions through proper bridging ligands to provide super exchange interaction. Morpholine complex materials are widely used in biomedical applications as this moiety serves as an important lysosome-targeting group. Some of its applications include synthesis lysosomes-targetable fluorescent probe for hydrogen sulfide imaging in living cells. Due to the attractive features of morpholine family crystals, we have synthesized a novel compound and reported. The title compound crystallizes in the monoclinic structure and $P21/n$ space group with 2 molecules in the unit cell. The unit cell parameters are $a = 8.6495(4) \text{ \AA}$, $b = 8.6593(4) \text{ \AA}$, $c = 13.1882(6) \text{ \AA}$, $\beta = 107.415^\circ$ and $V = 942.5 \text{ \AA}^3$. The grown crystals were subjected to study its optical, spectral and thermal properties by UV-Vis, FTIR and TG-DTA analysis respectively. Results will be discussed in detail.



ORTEP diagram of title compound

Green Synthesis of Silver Nanoparticles Using Leaf Extract and its Application in Photocatalytic Degradation of Dyes.

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ABSTRACT

The biogenic synthesis of silver nanoparticles (AgNPs) using leaf extracts at room temperature. The prepared AgNPs were characterized by UV-Visible spectroscopy, Fourier-transform infrared spectroscopy (FTIR), powder X-ray diffraction (XRD), Energy dispersive X-ray (EDX), High Resolution Transmission Electron Microscope (HRTEM), and Scanning Electron Microscopy (SEM). The bio reduction method is devoid of any toxic chemicals, organic solvents, and external reducing, capping and stabilizing agent. The synthesized AgNPs had spherical shape and had fcc structure. UV-Visible spectral analysis confirmed the formation of AgNPs with a characteristic surface plasmon resonance. The EDX pattern revealed the presence of elemental Ag in AgNPs. The prepared AgNPs were used for degradation of Fast green in aqueous medium, with efficiency within 15 min using 5 mg of AgNPs.

Keywords: Silver nanoparticles, Green bio synthesis leaf extract, Characterization, Dye degradation.

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**Exploring the Characterization and Biological Evaluation of a Carbazole-Pyrazole
Derivative as a Potential Tuberculosis Inhibitor**

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ABSTRACT

Tuberculosis (TB) remains a pressing global health challenge, demanding the continuous exploration of innovative drug candidates to combat this infectious disease. This study focused on the synthesis and evaluation of a compound that fuses a carbazole structure with a pyrazole ring, aiming to assess its potential as an effective TB inhibitor. The compound, referred to as the Carbazole-Pyrazole Derivative, was synthesized and characterized using X-ray Crystallography, which provided intricate details about its atomic arrangement and three-dimensional structure. This information is crucial for understanding its interactions with biological targets.

To comprehensively gauge the compound's pharmacokinetic properties and potential toxicity, we conducted an ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) evaluation. The results indicated satisfactory bioavailability and minimal toxicity risks, suggesting a favorable safety profile.

In order to delve deeper into the compound's binding interactions with the target protein associated with TB, we performed molecular docking studies. These docking results substantiated the compound's promise as a TB inhibitor by revealing its ability to establish favorable interactions within the binding pocket.

In summation, the findings of this research underscore the potential of the synthesized compound for further development as a promising therapeutic agent in the treatment of tuberculosis.

Keywords: ADMET, Crystal structure, Carbazole and pyrazole, DFT, drug-likeness, docking

Growth and Characterization of KTO Single Crystals for Optical Limiting Applications

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ABSTRACT

In nonlinear optics, optical power limiting (OPL) compounds are known to be an important class of materials because it has the ability to protect the optical sensor components as well as human eyes from the abrupt intense laser power. Here, we have grown such optical limiting material so called potassium trihydrogendioxalatedihydrate (KTO) single crystal from the aqueous solution by slow evaporation method at room temperature. The grown KTO single crystal results in triclinic crystal system with centrosymmetric space group $\overline{P1}$. The electronic band structure shows that KTO single crystal exhibits an insulating nature with band-gap energy of 3.436 eV (DFT). The strong observation of second harmonic generation (SHG) signal of 79 mV output from the centrosymmetric system is quite surprising and the efficiency of it is also almost equivalent to that of the standard KDP material. And this signal may be attributed due to the dehydration of the crystal under laser irradiation (centrosymmetric to non-centrosymmetric) and the third order nonlinear $\chi^{(3)}$ is found to be 1.82×10^{-6} esu. Apart from that, the material shows optical limiting behaviour at which it deviates from the linear response at 3.25 mW of input fluence (nonlinear origin) which further confirms that all nonlinear material will always be coupled with both linear and nonlinear property. In addition, optical, mechanical and dielectric properties of KTO single crystal are discussed in detail.

Comprehensive Investigation of 7-(5-benzyl-3H-indol-2-yl)-8-chloroquinoline as a Potential TMPRSS2 Inhibitor: Physicochemical Characterization and Molecular Docking Studies

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ABSTRACT

TMPRSS2 (Transmembrane Protease Serine 2) has arisen as a pivotal target for developing therapeutics against various viral infections, notably including SARS-CoV-2. This study focuses on exploring the physicochemical attributes and molecular interactions of a novel compound, 7-(5-benzyl-3H-indol-2-yl)-8-chloroquinoline, as a potential inhibitor of TMPRSS2.

The compound's physicochemical characterization leverages a range of computational tools and techniques. Molecular docking studies are conducted to predict binding affinity and interactions between the compound and the active site of the TMPRSS2 protein. Notably, the compound exhibits advantageous physicochemical properties, such as excellent solubility and drug-like characteristics, underscoring its potential as a drug candidate.

Molecular docking results unveil that the compound forms stable interactions with vital residues within the active site of TMPRSS2. These interactions encompass hydrogen bonding, hydrophobic associations, and π - π stacking, indicating robust binding affinity between the compound and the target protein. The analysis of the binding mode offers insights into the specific amino acid residues participating in these interactions, offering guidance for the rational design and optimization of TMPRSS2 inhibitors.

In summary, our findings underscore the promise of 7-(5-benzyl-3H-indol-2-yl)-8-chloroquinoline as a prospective TMPRSS2 inhibitor. Further validation through in vitro and in vivo studies is warranted to confirm its inhibitory activity and assess its therapeutic potential against viral infections, particularly with a focus on targeting TMPRSS2.

Keywords: TMPRSS2 inhibitor, Structure-based design, Molecular docking, Physicochemical Characterization.

Physicochemical Profiling and Molecular Docking Studies of N1-(7-Chloroquinolin-4-yl)-N1-(1H-Inden-2-yl)ethane-1,2-Diamine for Targeting SARS-CoV-2 Binding with ACE2

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ABSTRACT

The emergence and global dissemination of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) have spurred the urgent quest for effective therapeutic solutions. This study delves into the physicochemical attributes and potential binding interactions of a novel compound, N-(1H-benzo[d]imidazol-2-yl)-7-chloroquinolin-4-amine, concerning its interactions with the SARS-CoV-2 virus and its receptor angiotensin-converting enzyme 2 (ACE2).

Experimental techniques were employed for the physicochemical characterization of the compound, encompassing spectroscopic, elemental, and thermal analyses. The three-dimensional molecular structure was elucidated via X-ray crystallography, offering critical insights into its spatial arrangement and conformation.

Molecular docking simulations, utilizing cutting-edge software and considering compound and target protein structural information, probed potential binding interactions between the compound and the SARS-CoV-2 spike protein receptor-binding domain (RBD) as well as ACE2. Evaluation of binding affinity and key intermolecular interactions aimed to gauge the compound's efficacy as a SARS-CoV-2 inhibitor.

Preliminary findings unveiled favourable physicochemical properties in N-(1H-benzo[d]imidazol-2-yl)-7-chloroquinolin-4-amine, including stability and solubility, pivotal for drug development. Docking studies suggested the compound's capability to interact with the RBD of the SARS-CoV-2 spike protein, potentially impeding its binding to ACE2. Moreover, promising interactions with ACE2 hinted at a dual inhibitory mechanism against SARS-CoV-2.

These insights shed light on N-(1H-benzo[d]imidazol-2-yl)-7-chloroquinolin-4-amine as a potential therapeutic agent targeting SARS-CoV-2. Further validation through in vitro and in vivo studies is imperative to ascertain inhibitory efficacy and safety. This study contributes to the on-going endeavour for efficacious SARS-CoV-2 treatments, offering hope for the future management of COVID-19.

Keywords: Anticancer Activity, Structure-based design, Molecular docking, Physicochemical Characterization.

In Silico Exploration of Anticancer Potential, Physicochemical Profiling, and Molecular Docking Analysis of 4-(4-Chloro-2-(6-Chlorobenzo[d][1,3]dioxol-4-yl)phenyl)-3-Methyl-4H-1,2,3-Triazole

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ABSTRACT

Cancer continues to pose a substantial global health challenge, underscoring the need for on-going discovery of novel anticancer agents. This study employs In silico methodologies to investigate the potential anticancer activity, physicochemical attributes, and molecular docking interactions of a prospective compound, 4-(5-(6-chlorobenzo[d][1,3]dioxol-5-yl)cyclohexa-1,3-dien-1-yl)-4H-1,2,3-triazole.

The compound is subjected to in silico screening, assessing its potential to combat cancer across a spectrum of cancer cell lines using computational models. Its physicochemical properties, encompassing molecular weight, logP, and solubility, are scrutinized to evaluate its drug-like characteristics. Additionally, molecular docking analyses explore the interactions between the compound and selected protein targets associated with cancer pathways.

The In silico screening identifies the compound as a promising anticancer agent, displaying potent inhibitory effects against diverse cancer cell lines. Physicochemical profiling establishes its drug-like attributes, featuring optimal molecular weight and logP, endorsing its candidacy as a drug lead.

Molecular docking studies unveil specific binding interactions between the compound and crucial protein targets implicated in cancer progression and survival pathways. These interactions encompass hydrogen bonding, hydrophobic associations, and π - π stacking, signifying potential disruption of target proteins' functions and the interference with cancer-related signaling pathways.

In summation, our in silico explorations unveil the potential of 4-(5-(6-chlorobenzo[d][1,3]dioxol-5-yl)cyclohexa-1,3-dien-1-yl)-4H-1,2,3-triazole as an anticancer

candidate, underpinned by favorable physicochemical attributes and specific binding interactions with pertinent protein targets. These findings serve as a stepping stone for further experimental investigations, including in vitro and in vivo assessments, to validate its anticancer promise and enhance its structure for heightened efficacy and safety. The compound emerges as a promising frontrunner in the pursuit of innovative anticancer therapeutics.

Keywords: Anticancer Activity, Structure-based design, Molecular docking, Physicochemical Characterization.

Comprehensive Evaluation of Anti-HBV Activity: Structure-Based Design, Molecular Docking, and ADME/Pharmacokinetic Prediction Studies of 4-chloro-6-((5-methylbenzo[d][1,3]dioxol-2-yl)methyl)quinolone

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ABSTRACT

Hepatitis B virus (HBV) infection remains a global health challenge, necessitating the development of innovative antiviral agents. This study investigates the anti-HBV activity of a novel compound, 4-chloro-6-((5-methylbenzo[d][1,3]dioxol-2-yl)methyl)quinoline, employing a comprehensive approach that integrates structure-based design, molecular docking, and ADME/pharmacokinetic prediction studies.

The compound's structure was meticulously designed in accordance with rational drug design principles, featuring a quinoline framework and a 5,6-dimethoxybenzo[d][1,3]dioxol-2-yl moiety. Molecular docking studies were conducted to assess the binding affinity of the compound with pivotal HBV targets, including viral polymerase and capsid protein. The docking outcomes unveiled advantageous interactions between the compound and these target proteins, indicating potential inhibitory activity against HBV.

Furthermore, computational models were employed to predict the ADME (absorption, distribution, metabolism, and excretion) and pharmacokinetic properties of the compound. These predictions offered insights into the compound's oral bioavailability, tissue distribution, metabolic stability, and susceptibility to drug-drug interactions. The compound exhibited favourable ADME characteristics, signifying its suitability for further development as a potential anti-HBV agent.

In summary, our study establishes the anti-HBV activity of 4-chloro-6-((5-methylbenzo[d][1,3]dioxol-2-yl)methyl)quinoline, substantiated by the amalgamation of structure-based design, molecular docking, and ADME/pharmacokinetic prediction studies. These findings provide a foundation for the advancement of more potent and

selective compounds targeting HBV, setting the stage for forthcoming in vitro and in vivo investigations to validate its therapeutic promise.

Keywords: Anti-HBV Activity, Structure-based design, Molecular docking, Physicochemical Characterization.

Structural and optical properties of Zn doped Cobalt ferrite nanoparticles

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ABSTRACT

The hydrothermal approach was used to create the nanostructured zinc-doped cobalt ferrites. XRD, FTIR, UV-Vis, and FESEM, the produced nanoparticles were further characterized. Spinel ferrite's composition and structure were validated by XRD analysis. The nanoparticles' aggregated and spherical structure is verified by FE-SEM. FTIR was used to confirm the vibrational stretching modes of the tetrahedral (536 cm^{-1}) and octahedral (461 cm^{-1}) sites. The optical energy band gap proves that each sample contained visible active components.

Key words: XRD, FTIR, UV-Vis, FE-SEM, and Hydrothermal