National Seminar on

Emerging Material Science Research (NSEMSR 25)

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Organizing Secretaries
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Organized by
Department of Physics
Thiruvalluvar University,
Vellore-632 115.

National Seminar on Emerging Material Science Research (NSEMSR - 25)

12th March 2025

Seminar Proceedings

Convener

Dr. S. Uvarajan

Organized by

Department of Physics

Thiruvalluvar University,

Vellore

ISBN: 9789348505101

Published by

Royal Book Publishing
Ward No 10, Old No 118/07,
New No 52-1,
Ayothiyapattinam,
Salem.
Tamil Nadu-636103, India.
Email: contact@royalbookpublishing.com
Website: www.royalbookpublishing.com

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Vellore.

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திருவள்ளுவர் பல்கலைக்கழகம்

THIRUVALLUVAR UNIVERSITY

(State University Accredited with "B+" Grade by NAAC)

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 Seminar on Emerging Material Science Research (NSEMSR-25) on 12th March 2025, 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 NSEMSR-25 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

திருவள்ளுவர் பல்கலைக்கழகம்

THIRUVALLUVAR UNIVERSITY

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

MESSAGE

Warm and Happy greetings to all. I am immensely happy that the Department of Physics is organizing one-day National Seminar on Emerging Material Science Research (NSEMSR-25) on 12th March 2025.

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, Seminars and maintaining the research ambience in the Department.

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

Dr. J. Senthil Velmurugan
Registrar
Thiruvalluvar University

திருவள்ளுவர் பல்கலைக்கழகம்

THIRUVALLUVAR UNIVERSITY

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

MESSAGE

It gives me immense pleasure and pride to be a part of the National Seminar on Emerging Material Science Research (NSEMSR-25) on 12th March 2025 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 Seminar to create a platform for experts to share and learn.

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

Dr. R. Babujanarthanam

Controller of Examinations

Thiruvalluvar University

திருவள்ளுவர் பல்கலைக்கழகம்

THIRUVALLUVAR UNIVERSITY

(State University Accredited with "B+" Grade by NAAC)

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

MESSAGE

I am extremely happy to know that the Department of Physics, Thiruvalluvar University is organizing a one-day National Seminar on Emerging Material Science Research (NSEMSR-25) on 12th March 2025.

I believe that the seminar 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.

Dr. K. Dinakaran

Dean - Physical Science

Thiruvalluvar University

திருவள்ளுவர் பல்கலைக்கழகம்

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 National Seminar on Emerging Material Science Research (NSEMSR)-25.

It is very delightful to note that this seminar 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 seminar 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 of our Thiruvalluvar University for their support in the conduct of the one day National level Seminar on Emerging Material Science Research (NSEMSR) -25. Also, I thank the faculty members and students for their support to make this Conference a great success.

Dr. S. Uvarajan
Convener (NSEMSR)-25
Head (i/c), Department of Physics
Thiruvalluvar University

Invited Talks

1. Dr. E. Manikandan

Associate Professor

Centre for Nano Sciences & Technology

Pondicherry University

Pondicherry – 605 014, India.

2. Dr. W. Madhuri

Professor & Director

Centre for Functional Materials

Vellore Institute of Technology

Vellore - 632 014, Tamil Nadu, India.

National Seminar on Emerging Material Science Research (NSEMSR - 25)

(ISBN: 9789348505101)

IT-001

ADVANCES IN NANOMATERIALS SYNTHESIS PROCESS AND THEIR POTENTIAL APPLICATIONS

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ABSTRACT

Nowadays, advanced nanomaterials are increasingly recognized for their diverse applications across various fields, particularly in smart electronics, medicine (biomedical aspects), and environmental science. Their unique properties, such as high surface area, enhanced reactivity, and tunable optical characteristics, make them suitable for innovative solutions in numerous technological domains. In this context, transparent conducting metal oxides (TCMOs) such as Zinc Oxide (ZnO), Titanium Dioxide (TiO2), and Tin Dioxide (SnO2) are critical materials for various optoelectronic applications, including solar cells, sensors, and transparent electronics. This talk aims to explore various synthesis methods for these nanomaterials—such as laser ablation, ion implantation, electrochemical deposition, ion exchange, and traditional green routes—focusing on optimizing their properties to enhance performance in future technological applications.

Keywords: Advanced Materials; ZnO; TiO2; SnO2; Nanoparticles; Energy; Bio-medical Applications.

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National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

IT-002

COMPARISON OF LEAD BASED AND LEAD FREE PIEZOELECTRIC NANO GENERATORS FOR REAL TIME APPLICATIONS

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ABSTRACT

Ferroelectric ceramics are versatile in its application from electronic industry to medical applications. Ferroelectrics are good dielectrics and piezo electrics. The good texture of ceramics with controlled properties is important for the applications like energy conversion and storage. The literature review suggests no evidence of low sintering temperatures for different real-time applications. The dielectric ceramic capacitor stores electrical energy from electrostatic displacement caused by the electric field. Dielectric capacitors possess low energy and high power densities, the charge and discharge capability of dielectric capacitors are faster than batteries (less than 100 ns) (Jayakrishnan et al., 2019). Due to this reason the dielectric bulk ceramic capacitors are considered as energy storage devices for pulse power systems like electric vehicles, power grids etc (Qu et al., 2019). Most importantly, dielectric ceramic capacitors have a superior mechanical and thermal stability compare to batteries because it depends on polarization and depolarization in response to outside electrical fields instead of chemical reactions (Zou et al., 2019). This is essential for real-time energy storage application in pulse power systems.

Lead zirconium titanate (PZT) is the one most widely popular commercial electro-mechanical transducer. In the present research morphotropic PZT is synthesized by conventional solid- state ceramic route and is synthesized using microwave furnace. The sintering temperature and densification conditions are optimized by systematic sintering schedules. The PZT with morphotropic phase boundary and 95% theoretical density is obtained via hybrid microwave sintering. The PZT is studied for dielectric, ferroelectric and piezoelectric properties and further from the PE studies energy storage is estimated. The PZT nano powder is made in to a flexible

nano generator. Related testing and voltage generated are discussed.

Now a days, due to lead toxicity the research is directed towards lead free ferroelectrics. In order to explore lead free ferroelectrics and its potential for energy storage and conversion, Zr modified barium titanate (BT) is chosen. The modified barium titanate (BT) is synthesized along with zirconium oxide using microwave sintering. The dielectric and ferroelectric properties of the Zr modified BT are studied. These compositions are made in to nanofibers by electrospinng technique. These flexible fibers are used to prepare the nanogenerators. The peak voltages of nanogenerators are recorded. Further, proof of real-time applications are also incorporated.

Keywords*:* Hybrid Microwave Sintering; Electro- ceramics; Flexible Piezoelectric Nano generator; Electro Spinning Fibres; Energy Storage

References:

Jayakrishnan, A., Alex, K. V., Thomas, A., Silva, J., Kamakshi, K., Dabra, N., Sekhar, K., Moreira, J. A. and Gomes, M. (2019), 'Composition-dependent xba (zr0. 2ti0. 8) o3-(1-x)(ba0.7ca0. 3) tio3 bulk ceramics for high energy storage applications', Ceramics International 45(5), 5808–5818.

Zou, K., Dan, Y., Xu, H., Zhang, Q., Lu, Y., Huang, H. and He, Y. (2019), 'Recent advances in lead-free dielectric materials for energy storage', Materials Research Bulletin 113, 190–201.

(ISBN: 9789348505101)

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(ISBN: 9789348505101)

A-001

SPECTROSCOPIC, PHYSICAL, CHEMICAL, BIOLOGICAL AND MOLECULAR DOCKING INVESTIGATIONS OF DFT APPROACH AN ANTIDEPRESSANT AGENT

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ABSTRACT

Experimental and theoretical studies on the optimized geometrical structure, electronic and Vibrational characteristics Doxepin are presented employing B3LYP/6-311++G (d,p) basis set. Simulated FT-IR and FT-Raman spectra were in concurrence with the observed spectra attained in a spectral range of FT-IR (4000 - 400 cm-1) and FT-Raman (4000 - 100 cm-1). Quantum chemical calculations and the comprehensive Vibrational assignments of wavenumber of the optimized geometry using Potential Energy Distribution (PED) were calculated with scaled quantum mechanics. Theoretical UV-Visible spectrum was obtained in different solvents and in gas phase using TD-DFT method. The calculated HOMO and LUMO energies show that charge transfer within the headline molecule. Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital analysis (NBO). In addition, MEP map was traced to find the reactive sites of molecule. Further, NLO properties such as dipole moment, linear and first order hyperpolarizability have been studied to reveal NLO nature of the title compound. ELF, LOL, and RDG were implemented using topological assessment for gas phases and solvents. Molecular docking (ligand-protein) studies were made on the title compound to study the hydrogen bond interactions and the minimum binding energy was calculated.

Keywords: DFT; FT-IR; FMO; NLO; NBO; Docking

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-002

STUDIES ON DYES DOPED ADP CRYSTALS FOR POSSIBLE LASER APPLICATIONS

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ABSTRACT

In present work Ammonium Didydrogen phosphate (ADP) crystal are one of the most popular crystal used for Non-linear optical (NLO) application. Pure and dye (Allura Red) doped ADP crystal were grown by slow evaporation technique at room temperature. The properties of the crystal have been improved by doping of inorganic impurities. In the present investigation, Pure and dyes (Allura Red) doped ADP crystals are verified by FTIR, UV and NLO analysis. The optical nature of the grown crystal is analyzed using the UV-Vis spectrum. The UV-Visible spectrophotometer is used to determine the absorption or transmission of light by a sample. The presence of the functional groups has been identified by Fourier Transform Infrared spectrum (FTIR). The infrared absorption bands identify molecular components and structures. In Vicker's microhardness analysis the mechanical properties of doped crystal are increased compared with pure ADP crystals. The NLO reports of the samples are having high energy level comparing with pure ADP. A variety of dyes for many laser operating wavelengths were employed in the past. Dye embedded in ADP crystal and dye doped crystal were also reported as useful non-linear optical media.

Key words: ADP Crystal, FTIR Studies, UV Studies, Micro hardness, NLO studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-003

CHARACTERIZATION STUDIES ON DYES DOPED KDP CRYSTALS

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ABSTRACT

Potassium Dihydrogen Phosphate (KDP) doped with dyes and it has been grown by slow solvent evaporation method at room temperature. The properties of the crystal have been improved by doping of impurities. In the present investigation, Pure and dyes (Biebrich Scarlet) doped KDP crystals are verified by FTIR, UV and Microhardness analysis. The optical nature of the grown crystal is analyzed using the UV-Vis spectrum. The UV-Visible spectrophotometer is used to determine the absorption or transmission of light by a sample. The presence of the functional groups has been identified by Fourier Transform Infrared spectrum (FTIR). The infrared absorption bands identify molecular components and structures. In Vicker's microhardness analysis the mechanical properties of doped crystal are increased compared with pure KDP crystals.

Key words: Crystal growth, KDP crystals, Dyes, FTIR Studies, UV studies, Microhardness Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-004

OPTIMIZED HEMATITE ANODES: UNLOCKING SUPERIOR LITHIUM-ION STORAGE WITH MOS_2 DOPING

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ABSTRACT

This study investigates the electrochemical enhancement of hematite (Fe_2O_3) as an anode material for lithium-ion batteries through molybdenum disulfide (MoS_2) doping. The Fe_2O_3-MoS_2 composite exhibits remarkable improvements in lithium-ion storage performance compared to pure hematite. The integration of MoS_2 enhances electrical conductivity and effectively addresses hematite's intrinsic limitations, including low electronic conductivity and significant volume expansion during charge-discharge cycles. With superior rate capability and cycling stability, the composite emerges as a strong contender for next-generation lithium-ion battery anodes. This research underscores the synergistic effects of Fe_2O_3 and MoS_2 in revolutionizing energy storage technology.

Keywords: Electrochemical, Cycling Stability, Energy Storage, Anode Material**.**

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-005

INVISTIGATION ON DYES DOPED KDP CRYSTALS FOR NLO APPLICATION

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ABSTRACT

Potassium Dihydrogen phosphate (KH_2PO_4) is a well-known inorganic crystals. It has a transparent dielectric material best known for its non-linear optical and electro optical properties. The KDP crystal has wide frequency conversion, high damage threshold against power laser and good UV transmission. It has been incorporated into various laser systems for harmonic generation, opto electrical switching etc., Tartrazine dye has been and desired to dope in KDP. In present study single crystal of pure and Tartrazine doped KDP has been grown by slow evaporation solution growth technique. Crystal growth is dependent on temperature. The enhancement in transmittance of grown KDP crystal with Tartrazine was analysis by UV-visible spectral analysis. The FT-IR spectrum analysis is carried out for pure and doped crystals. The mechanical properties of the grown crystal are analyses by Vicker's microhardness studies. In Vicker's microhardness analysis the mechanical properties of doped crystal are increased compared with pure KDP crystals.

Key words: KDP Crystal, FTIR Studies, UV studies, NLO Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-006

METAL-ORGANIC FRAMEWORKS FOR NEXT-GENERATION SUPERCAPACITORS

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ABSTRACT

Metal-Organic Frameworks (MOFs) have emerged as a groundbreaking class of porous materials with immense potential for next-generation supercapacitors. These materials consist of metal ions or clusters coordinated with organic linkers, resulting in highly tunable structures with exceptional surface areas, controlled pore sizes, and diverse functionalities. Unlike conventional porous carbon-based materials, MOFs offer the unique advantage of customizable architecture, allowing for the fine-tuning of their electrochemical properties. The high porosity and large surface area of MOFs enhance ion diffusion and charge storage capacity, making them highly suitable for supercapacitor applications. Additionally, their structural diversity enables the incorporation of various electrochemically active metal centers, which contribute to faradaic charge storage, thus improving capacitance beyond the capabilities of traditional electrical double-layer capacitors (EDLCs). One of the major advantages of MOFs in supercapacitor applications is their ability to undergo post-synthetic modifications. By carefully selecting metal nodes and organic linkers, researchers can introduce functional groups that enhance electrical conductivity and electrochemical stability. Furthermore, composite materials derived from MOFs, such as MOF-derived carbon or MOF-based hybrids with conductive polymers and metal oxides, have demonstrated remarkable improvements in energy and power density. These composites leverage the intrinsic properties of MOFs while overcoming their inherent limitations, such as low electrical conductivity. Another critical aspect of MOFs in supercapacitors is their role in pseudocapacitive charge storage mechanisms. Unlike EDLCs, which rely purely on electrostatic charge accumulation at the electrode-electrolyte interface, pseudocapacitors exploit fast and reversible redox reactions for energy storage. MOFs, particularly those containing transition metal centers like cobalt, nickel, or manganese, exhibit

significant pseudocapacitive behavior, thereby enhancing their overall energy storage capability. Moreover, the integration of conductive elements, such as graphene or carbon nanotubes, with MOFs has led to hybrid materials that combine the high capacitance of MOFs with the excellent conductivity of carbon-based nanomaterials. This synergistic combination addresses the primary drawback of pristine MOFs, which is their relatively low electrical conductivity. The advent of MOF-derived porous carbon materials has further expanded the application of MOFs in supercapacitors. By subjecting MOFs to controlled pyrolysis, researchers can obtain highly porous carbon structures with well-preserved morphologies and enhanced conductivity. These MOF-derived carbons exhibit superior electrochemical performance, with high capacitance retention and excellent cycling stability. Additionally, doping these carbon frameworks with heteroatoms such as nitrogen, sulfur, or phosphorus has been shown to improve electrochemical activity and charge storage characteristics. The future of MOF-based supercapacitors lies in addressing challenges such as structural stability, scalability, and cost-effectiveness. While MOFs exhibit outstanding electrochemical properties, their practical application requires further improvements in mechanical stability and long-term cycling performance. Moreover, the synthesis of MOFs at an industrial scale remains a challenge due to the high cost of precursors and complex fabrication processes. Research efforts are focused on developing scalable synthesis methods, including green and cost-effective approaches, to make MOFs commercially viable for energy storage applications. The integration of MOFs with flexible and wearable electronics is also an emerging area of interest, paving the way for their use in next-generation energy storage devices. As advancements in material design, synthesis, and engineering continue, MOFs hold great promise for revolutionizing the field of supercapacitors, offering a sustainable and high-performance alternative for energy storage in modern technological applications.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-007

STUDIES ON MECHANICAL PROPERTIES OF DYES DOPED ADP CRYSTALS

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ABSTRACT

Ammonium Dihydrogen phosphate (ADP) crystals are one of the most popular crystals used for Non-linear optical (NLO) applications. Pure and dye (Bismarch Brown) doped ADP crystals were grown by slow evaporation technique at room temperature. Grown crystals have been characterized using Fourier Transform Infrared Spectroscopy (FTIR). The presences of dyes were confirmed by FTIR and UV-visible spectra. Dye molecules possess π electron similar to conjugated polymers, but the molecules themselves are not very big. Their energy level structure shows the presence of bands containing many closely spaced levels corresponding to vibrational and rotational states. The analysis of single crystal FTIR and UV spectra conforms that the doped sample has the perfect crystal properties. Their energy level structure shows the presence of bands containing many closely spaced levels corresponding to vibrational and rotational states. A variety of dyes for many laser operating wavelengths were employed in the past. The Vicker's hardness studies carried out for the Pure and doped crystals from the crystallographic planes. It shows that an increased hardness of the doped crystals with comparison of pure ADP.

Key words: ADP Crystal, FTIR Studies, UV Studies, Microhardness studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-008

CHARACTERIZATION STUDIES ON DYES DOPED ADP CRYSTALS

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ABSTRACT

Ammonium Dihydrogen Phosphate (ADP) is a well known inorganic crystals. It has a transparent dielectric material best known for its non-linear optical and electro optical properties. The ADP crystal has wide frequency conversion, high damage threshold against power laser and good UV transmission. It has been incorporated into various laser systems for harmonic generation, opto electrical switching etc., Biebrich Scarlet dye has been and desired to dope in ADP. In present study single crystal of pure and Biebrich Scarlet doped ADP has been grown by slow evaporation solution growth technique. Crystal growth is dependent on temperature. The Vicker's hardness studies carried out for the Pure and doped crystals from the crystallographic planes. It shows that an increased hardness of the doped crystals with comparison of pure ADP. The enhancement in transmittance of grown ADP crystal with Biebrich Scarlet was analysis by UV-visible spectral analysis. The FT-IR spectrum and X-ray diffraction analysis are carried out for pure and doped crystals.

Key words: ADP Crystal, UV analysis, FTIR Studies, Microhardness Studies.

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(ISBN: 9789348505101)

A-009

FT-IR STUDIES ON THE MOLECULAR MAGNET PRUSSIAN BLUE, IRON (III) HEXACYANOFERRATE(II) ($FE_4[FE(CN)_6]_3.14H_2O$)

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ABSTRACT

Molecular magnet is an emerging field of magnetism that has more nano-technological applications especially in molecular spintronics, quantum technologies, metal–organic frameworks (MOFs) and 2D materials. We report here, FT-IR studies on nano crystalline Prussian blue, Iron (III) Hexacyanoferrate(II) ($Fe_4[Fe(CN)_6]_3.14H_2O$), a molecular magnet that was synthesized by solution precipitation method at room temperature. The results showed clearly the typical functional groups belonging to Prussian blue. when compared with the ones that are available in the literature[3,4].

Keywords: Molecular magnets, Nanocrystals, FT-IR.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-010

INVISTIGATION ON DYES DOPED ADP CRYSTALS FOR NLO APPLICATION

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ABSTRACT

Tartrazine azo dye was doped with ADP were grown by slow evaporation growth technique. It is well known that Ammonium dihydrogen phosphate (ADP) crystals are one of the most popular crystals used for non-linear optical application. In the present work, the Tartrazine doped ADP crystals are subjected in to various techniques. In present study single crystal of pure and Tartrazine doped ADP has been grown by slow evaporation solution growth technique. Crystal growth is dependent on temperature. The optical properties of the grown crystals are analysis through UV-visible spectrum. The doping of Tartrazine in ADP crystal is confirmed by FT-IR spectroscopy studies. A variety of dyes for many laser operating wavelengths were employed in the past. The NLO reports of the samples are having high energy level comparing with pure ADP. Dye embedded in ADP crystal and dye doped crystal were also reported as useful non-linear optical media.

Key words: ADP Crystal, UV analysis, FTIR Studies, NLO Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-011

GROWTH AND CHARACTERIZATION OF GLYCINE AND AMMONIUM ACCETATE BY SLOW EVAPORATION METHOD

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ABSTRACT

Gamma Glycine single crystal is a potential organic nonlinear optical (NLO) material. It has been grown from a mixture of aqueous solutions of Glycine and Ammonium acetate by slow evaporation solution growth technique at room temperature for the first time. The grown crystals have been exposed to various characterization techniques such as single crystal / powder XRD, UV- Vis- NIR absorption, FTIR, thermal analysis and powder SHG measurements. The powder XRD analysis confirms the grown crystal is subjected to "TETRAGONAL" system. The UV-visible spectrum shows there is no absorption of light in the visible region. It shows in the visible region 100% transparent also in the transmittance spectrum. The cut off wavelength is 202 nm. The GAA crystal was recorded in KBr phase in the frequency range 500 - 400 cm-1using FTIR- 8400S spectrometer.

Key words: XRD, UV- Vis, FTIR and Thermal Analysis.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-012

GROWTH AND CHARTERIZATION STUDIES OF DOPED THIOUREA CRYSTALS

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ABSTRACT

The technology strength of the nation the key to reach this developed status in fluency of doping the Allura Red in Thiourea crystals grown by slow evaporation room temperature method has been investigated. The concentration of dopants in the mother solution with Allura Red for Thiourea solution were obtained with well-defined characterization of the grown crystals were carried out by single crystal FTIR and UV analysis. The FT-IR spectra study reveals the presence of ruinous functional groups and confirms the slight distortion of the structure of the crystal due to doping. The UV-visible spectra study was carried out to analysis the optical transmittance of the obvious regions for both pure and doped crystals. The hardness of the pure and doped crystals is studies by using Vicker's tester. The Vicker's hardness studies carried out for the Pure and doped crystals from the crystallographic planes. It shows that an increased hardness of the doped crystals with comparison of pure Thiourea.

Key words: Thiourea Crystal, UV analysis, FTIR Studies, Microhardness Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-013

CHARTERIZATION STUDIES OF DOPED THIOUREA CRYSTALS FOR NLO APPLICATIONS

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ABSTRACT

The influence of doping the Biebrich Scarlet on pure Thiourea grown by the slow evaporation method has been investigated. The concentration of Biebrich Scarlet dopent in the mother solution with 0.01g for Biebrich Scarlet was carried out individually and crystals were obtained with well defined morphology. In present study single crystal of pure and Biebrich Scarlet doped Thiourea has been grown by slow evaporation solution growth technique. Crystal growth is dependent on temperature. The FTIR spectral study reveals the presence of various functional groups and confirms the slight distortion of the structure of the crystals due to doping. The UV-visible spectral study was carried out to analysis the optical transmittance of the grown crystals and found that the transmittance is very high in visible and UV regions for both pure and doped crystals. The NLO reports of the samples are having high energy level comparing with pure Thiourea. Dye embedded in Thiourea crystal and dye doped crystal were also reported as useful non-linear optical media.

Key words: Thiourea Crystal, slow evaporation technique, UV analysis, FTIR Studies, NLO Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-014

AUTOMATIC STREET LIGHT CONTROLLER USING LDR AND ARDUINO

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ABSTRACT

Automation is a significant aspect of modern urban infrastructure, enhancing efficiency, reducing resource wastage, and promoting sustainability. This project focuses on the development and implementation of an Automatic Street Light Control System using a Light Dependent Resistor (LDR), Arduino microcontroller, and LED technology. The objective is to create a cost-effective and energy-efficient solution for controlling streetlights, ensuring they operate only when required.

The system employs the LDR as a light sensor to detect ambient light levels. When the surrounding light intensity falls below a predetermined threshold—such as during nighttime—the system automatically switches the streetlights on. Conversely, the lights turn off as daylight resumes, thereby eliminating manual intervention and reducing power consumption.

The use of Arduino facilitates precise control and decision-making in response to real-time light conditions. A simple yet robust circuit design incorporating a 4.7kΩ resistor, breadboard, and connecting wires integrates the hardware components seamlessly. The implementation also includes programming the Arduino to interpret data from the LDR and activate or deactivate the LEDs accordingly.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-015

OPTICAL AND MECHANICAL PROPERTIES OF DYES DOPED THIOUREA CRYSTALS

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ABSTRACT

Thiourea crystal is a popular non-linear optical inorganic material. In my present investigation, Thiourea crystal and Bismarch Brown doped crystal has been grown by slow evaporation at room temperature growth technique. The grown crystals have been analysis through various viz. Fourier Transform Infrared spectroscopy has been used for spectral analysis of grown crystals. The crystals are subjected into UV analysis. The UV-visible spectra study was carried out to analysis the optical transmittance of the obvious regions for both pure and doped crystals. The hardness of the pure and doped crystals is studies by using Vicker's tester. The Vicker's hardness studies carried out for the Pure and doped crystals from the crystallographic planes. It shows that an increased hardness of the doped crystals with comparison of pure Thiourea. Using Vicker's microhardness test the mechanical properties of Thiourea crystal and Bismarch Brown doped Thiourea has been studied.

Key words: Thiourea Crystal, Slow evaporation method, UV analysis, FTIR Studies, Microhardness Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-016

MINERALOGICAL ANALYSIS AND ELASTIC PROPERTY FOR DIFFERENT IDOL MAKING ROCKS FTIR STUDY

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ABSTRACT

In this study, it is aimed to find out the composition of minerals of some rock samples Collected at idol making rocks using FTIR Spectroscopy and to study the Elastic properties of rock samples using Ultrasonic Investigations. Rock samples were collected from different hill region at. Totally 10 samples were collected. All the 10 samples were finely ground to powder. The ground powders were mixed with KBr in proper ratio and pellets were prepared. The KBr pellets were subjected to IR radiations in a FTIR Spectrometer and absorption spectra were recorded. From the available literature, minerals such as quartz, feldspar in different structures (microline and orthoclase), kaolinite, montmorillonite and organic carbon were identified in the rock samples and they are listed. The rock samples were suitably cut and subjected to Ultrasonic investigation.through Pulse Echo Technique. The elastic properties such as Young's modulus, Bulkmodulus and Shear modulus were calculated and tabulated using the calculatedlongitudinal and shear velocities of Ultrasonic waves through the rock samples. From the mineral composition and elastic properties, it is aimed for further FTIR studies in future scope.

Keywords: FTIR – Study, ultrasonic investigation, elastic property, mineral analysis.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-017

TRAFFIC LIGHT CONTROL SYSTEM USING AN ARDUINO MICROCONTROLLER

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ABSTRACT

Traffic congestion and ineffective traffic control systems are pressing challenges in modern urban environments. To address these issues, this project presents the design and implementation of a Traffic Light Control System using an Arduino microcontroller. This beginner-friendly system replicates the standard traffic light sequence—red, yellow, and green lights—offering an automated and low-cost solution for managing traffic flow at intersections.

The primary objective of this project is to provide a practical and educational approach to understanding the fundamentals of embedded systems and automation. By utilizing an Arduino microcontroller, LEDs, and resistors, the project demonstrates how programmable systems can automate everyday tasks with efficiency and precision. The system follows a predefined sequence to control the lights, ensuring seamless and accurate transitions between traffic signals. This simulation aligns with real-world traffic light operations and highlights the potential for future enhancements such as vehicle detection or adaptive timing.

The implementation focuses on simplicity, making it an ideal project for beginners in electronics and programming. Through this system, users gain hands-on experience in assembling circuits, coding in Arduino IDE, and understanding the functionality of microcontroller-based automation. In addition, the energy efficiency of LEDs and the modular design of the system make it suitable for practical applications and further scalability.

National Seminar on Emerging Material Science Research (NSEMSR - 25)

(ISBN: 9789348505101)

A-018

INVESTIGATING THE IMPACT OF SOLUTION AND MOLECULAR STRUCTURE ELUCIDATIONHEXADECANAMIDE'S QUANTUM COMPUTATIONAL CHARACTERISTICS AND BIO ACTIVITY ANALYSIS.

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ABSTRACT

The Hexadecanamide (HDA) was examined using spectroscopic techniques such as FT-IR. DFT analysis was also utilized to clarify the procedures for determining electronics-MAsed transmissions in the UV-Vis spectral region of different solvents. The quantum chemistry simulation calculations were carried out using a flexible MAsis set -B3LYP/6-311++G(d,p) technique. We calculated the maximum wavelength (λ) absorMAnce and MAnd-gap energy estimates for HDA for a range of solvents. Molecular interactions with solvents were investigated using UV- visible, HOMO-LUMO, MEP, and NBO properties. According to these findings, there are some differences in the chemical activity in the solvent and gas phases. Using the Multiwfn software, topological studies have shown the nucleophilic and electrophilic regions, including active sites. Completed characterizations of the theoretical and experimental spectrums revealed a reasonable connection between the experimental value and the vibrational wavenumbers. The topological studies of LOL, ELF, and RDG were performed. The drug-active molecule's features are due to the hydrophobic (water-repelling) properties of the long alkyl chain.

Key words: FTIR, UV, HOMO-LUMO, MEP and NBO properties.

(ISBN: 9789348505101)

A-019

SPECTROSCOPIC CHARACTERIZATION AND NATURAL BOND ORBITAL ANALYSISOF MASED ON DFT CALCULATIONS

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ABSTRACT

The experimental Fourier transform infrared (FT-IR) and Fourier transform Raman (FT-Raman) spectra of 4-cyanopyridine have been recorded in the spectral region 4000-400cm -1 and 3500-100cm -1 , respectively. Also, the title molecule has been characterized by 13C NMR and 1H NMR spectroscopes. The geometry optimization and frequency calculations have been performed at B3LYP/6-311+G(d,p), and 6-311++G(d,p) level. A detailed interpretation of FT-IR and FT-Raman Spectra aided by the potential energy distributions (PEDs) for the calculated frequencies has been reported. Results of this study showed that there is a good correlation between experimental and computational results. The HOMO-LUMO energy gap explains the charge transfer interaction's in the molecule. NBO (natural bond orbital) computations have been utilized to evaluate the stabilities which occur from charge delocalization and inter-molecular interactions have been studied using DFT calculations.

Key words: FT-IR, FT-Raman, NMR, PED, NBO.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-020

PREPARATION AND CHARACTERIZATION OF P-TYPE CU DOPED NIO THIN FILMS BY SPIN COATING TECHNIQUES

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ABSTRACT

Pure and Cu-doped NiO thin films were deposited on glass substrate by sol gel homemade spin coating method from nickel(II) acetate tetrahydrate (Ni(OCOCH 3) 2 .4H 2 O) (98% Sigma Aldrich), copper(II) acetate monohydrate (Cu(CO 2 CH 3) 2 .H 2 O) (≥99% Sigma Aldrich), 2- methoxyethanol and monoethanolamine. The XRD spectrum of NiO thin films with different molar ratio of Cu. All the diffracted peaks matched well with the standard JCPDS card No. (65-2901 and 47- 1049) and attributed to crystalline nature without any impure phase indicating that Cu atoms incorporated in NiO lattice, implies that the structure of the films were not affected due to the addition of Cu. Optical band gap energy was found to be decreases in the range of 3.78, 3.74, 3.71 and 3.66 eV for pure and Cu doped NiO thin films due to increase crystalline quality and grain size. DC electrical conductivity studies reveals that the current increases with increase of voltage for pure and different concentration of Cu. SEM results can be observed that the structure of NiO thin films formed in spherical shape at 3% of Cu concentration.

Keywords: NiO thin films, Grain size, Electrical conductivity, Band gap energy

(ISBN: 9789348505101)

A-021

EXPERIMENTAL (FT-IR, FT-RAMAN AND UV-VIS) AND QUANTUM CHEMICALCALCULATIONS ON MONOMER AND DIMER STRUCTURES OF PICOLINIC ACID USING THE DFT AND TD-DFT METHODS

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ABSTRACT

The quantum chemical calculations and FTIR and FT-Raman characterization of picolinic acid have been recorded in the regions 4000-400 cm -1 and 3500-400 cm -1 respectively, Employing the experiential FT Raman and FTIR data, a complete vibrational assignments and analysis of the fundamental modes of afterward confirmed by total energy distribution (TED s) in the calculations achieved to determine the optimum molecular geometry, harmonic vibrational frequencies, infrared intensities and Raman scattering activities, the density functional theory (DFT/B3LYP) method with 6-31++G(d,p) and 6- 311++G(d,p) MAsic sets have been compared with the experimental values the difference between the observed and scaled wavenumber values of most of the vibrational modes is very small, The effects of frontier, orbitals HOMO and LUMO and the transition of electron density transfer have been discussed. The UV-Vis spectrum has been done which confirms the charge transfer. The chemical interpretation of hyper conjugative and charge delocalization has been analysed using natural bond orbital (NBO) analysis, Structure MAsed Molecular docking studies of picolinic acid Target protein Taurine dehydrogenase inhibitor.

Keywords: DFT, HOMO, LUMO, Taurine dehydrogenase, picolinic acid.

(ISBN: 9789348505101)

A-022

SYNTHESIS AND EVALUATION OF NOVEL ANTICANCER COMPOUNDS DERIVED FROM THE NATURAL PRODUCT MORUS ALMA

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ABSTRACT

Cancer is the second leading cause of death gloMAlly, responsible for an estimated 9.6 million deaths in 2018, and this burden continues to increase. Therefore, there is a clear and urgent need for novel drugs with increased efficacy for the treatment of different cancers. Previous research has demonstrated that morus alma exerts anticancer activity in various cancers, including human multiple myeloma, breast cancer, lung cancer, and colon carcinoma, suggesting the anticancer potential present in the chemical scaffold of **MA**. Here, we designed and synthesized a small library of 12 novel MA derivatives and evaluated the biological anticancer effects of the compounds in various cancer cell lines. The results of this structure–activity relationship study demonstrated that MA derivatives **MA-9** and **MA-10** possessed significantly improved anticancer activity toward lung, colon, and breast cancer cell lines. **MA-9** and **MA-10** could more effectively reduce cancer cell viability and induce DNA damage, cell-cycle arrest, and apoptosis when compared with **MA**. Our findings represent a significant step forward in the development of novel anticancer entities.

Keywords: FTIR, Photochemical screening, GC-MS analysis.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-023

FTIR SPECTROSCOPIC STUDIES ON RIVER SEDIMENT SAMPLES FROM SATHANUR DAM, THIRUVANNAMAI DISTRICT, TAMILNADU, INDIA.

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ABSTRACT

The river sediment samples from sathanur dam thiruvannamai districtis subjected to mineral analysis. FTIR spectroscopic technique is applied to sediment samples to identify the constituent minerals. From the infra spectrum, the minerals are identified from the location or MAnd position of peaks with the help of available literature. The minerals such as quartz, orthoclase, microcline, albite, kaolinite, montmorlinite, calcite, aragonite and organic carbon are identified. The performed analyses provided useful information about the mineralogical composition of the sediments. FT-IR spectroscopy seems to be useful method for the mineral analysis of River sediments.

Keywords: River sediment, Mineral Analysis, FT-IR technique.

A-24

ENHANCED ON ELECTRICAL CONDUCTIVITY OF CO:AL CO-DOPED ZNO THIN FILMS VIA SOL-GEL SPIN COATING METHOD

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ABSTRACT

In this research work, Cobalt doped AZO thin films has been deposited on glass substrate via sol-gel spin coating technique and the precursors are Zinc acetate dehydrate, Aluminum nitrate nonahydrate and Cobalt acetate dehydrate respectively. Various concentration of Cobalt co-doped AZO thin films were annealed at 550°C for 2 hrs. XRD results show the crystalline structure of pure and co-doped ZnO thin films and confirmed the formation of hexagonal wurtzite structures. Nanoparticles ranging from 35-50 nm are found from the SEM results. The optical transmittance and absorbance of all ZnO thin films decreased with the increase of cobalt concentrations.

Keywords: ZnO thin films, concentrations, co-doped, spin coating, nanoparticles

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-025

FTIR SPECTROSCOPIC STUDIES ON COSTAL SEDIMENT SAMPLES FROM MARAKANAM, VILLUPURAM DISTRICT, TAMILNADU, INDIA.

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ABSTRACT

The Costal sediment samples from Costal sediment samples from Marakanam Villupuram district subjected to mineral analysis. FTIR spectroscopic technique is applied to sediment samples to identify the constituent minerals. From the infra spectrum, the minerals are identified from the location or MAnd position of peaks with the help of available literature. The minerals such as quartz, orthoclase, microcline, albite, kaolinite, montmorlinite, calcite, aragonite and organic carbon are identified. The performed analyses provided useful information about the mineralogical composition of the sediments. FT-IR spectroscopy seems to be useful method for the mineral analysis of River sediments.

Keywords: Costal sediment, Mineral Analysis, FT-IR technique.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-026

EFFECT OF AL DOPED ON MICROSTRUCTURAL, MORPHOLOGICAL AND OPTICAL PROPERTIES OF ZNO NANO RODS

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ABSTRACT

In this paper, one dimensional ZnO nanorods are grown with the synthesis of ZnO seed layers are deposited on glass substrate by sol gel spin coating technique using zinc acetate dehydrate $(CH_3COO)_2Zn.2H_2O$, 2-methoxyethanol and monoethanolamine followed by the growth of zinc oxide nanorods on the seed layer by hydrothermal process with zinc nitrate $(Zn(NO_3)_2.6H_2O)$ and Hexamethylenetetramine (HMT). The structural, surface morphology, electrical and optical properties has been analyzed with the results obtained from X-Ray diffraction study, Field Emission Scanning Electron Microscopy (FESEM) and UV-Visible spectroscopy respectively. Results of XRD confirmed the hexagonal wurtzite ZnO nanorods having the orientation of (002) plane. Al (concentration of Al viz., 2%, 4%, 6% and 8%) is used to dope ZnO nanorods. Results revealed that, the results increase in the concentration of Al dopant has influenced the optical band gap i.e., decreases compared to the pure ZnO. The optical band gap for various Al concentration are 3.10, 3.06, 3.04 and 3.01 eV and 3.15eV for pure ZnO nanorods.

Key words: ZnO nanorods, seed layers, hydrothermal process, thin films

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-027

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING MANGO GINGER AND INVESTIGATION OF THEIR ANTIBACTERIAL ACTIVITIES

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ABSTRACT

This study aimed to develop an environmentally friendly and cost-effective approach to synthesize green silver nanoparticles (gNPs) from silver precursors. Green synthesis of AgNPs was accomplished using the aqueous extract of **mango ginger**, in which plant biomaterials were used as a reducing as well as a capping agent. After 24 h of reaction, the yellow color of the extract was changed to dark brown-reddish due to the reduction of silver ions to AgNPs. AgNPs were characterized using UV–vis spectroscopy, Fourier transform infrared spectroscopy, transmission electron microscopy (TEM), and energy dispersive X-ray spectroscopy (EDS). The maximum absorbance of the UV–vis spectra was at 432 nm. TEM analysis reveals that the shape of most of the biosynthesized AgNPs was spherical forms and the average particle size was 18 ± 0.5 nm. EDS analysis exhibits strong signals of silver element. In addition, green synthesized AgNPs show high and efficient antimicrobial activities against two food-borne pathogens (*Escherichia coli* O157:H7 and *Listeria monocytogenes*). TEM and scanning electron microscopic images reveal that there were significant shrinkage and damage of bacterial cell wall, and leakage or loss of bacterial intracellular contents. A significant reduction ($P \leq 0.05$) of bacterial counts just after 4 h of exposure was observed. These results indicate that green synthesized AgNPs can be utilized as an antimicrobial means to inhibit the growth of pathogenic bacteria for applications in agricultural and food industries.

Keywords: Green synthesis, Nanoparticles, Microstructral analysis, TEM, FTIR

National Seminar on Emerging Material Science Research (NSEMSR - 25)

(ISBN: 9789348505101)

A-028

SYNTHESIS AND CHARACTERIZATION OF TIO_2 NANOPARTICLES WITH ENHANCED ANTIBACTERIAL ACTIVITY

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ABSTRACT

In this study, TiO_2 nanoparticles were synthesized using the sol-gel method. The crystal structure, morphology, optical properties, and chemical composition of the synthesized nanoparticles were characterized by using XRD, SEM, HR-TEM, and UV-vis spectroscopy. The average crystallite sizes of the TiO_2 were approximately 15.2 nm, respectively. Particle size is affected by the nature of the surfactant. Spherically shaped nanoparticles with aggregation and a homogeneous size distribution were observed using SEM and HR-TEM. The bandgap was determined to be 3.24 eV and was found to have excellent optical behavior.

Keywords: TiO_2 nanoparticles, sol-gel, morphology, and antibacterial activity

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-029

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING PLANT ROOT EXTRACTION OF MIMOSA PUDICA ROOT POWDER

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ABSTRACT

Green synthesis of metal nanoparticles using plant extract is an eco-friendly and cost-effective method for synthesizing metal nanoparticles. In this present work silver nanoparticles have been synthesized using ethanolic extract of Mimosa Pudica root powder Linn plant (MPL) leaves. Green synthesized silver nanoparticles (AgNps) have been characterized by UV-Vis spectrometer, Fourier Transform Infra-Red ((FTIR) spectra, dynamic light scattering (DLS), Scanning Electron Microscopy (SEM) and X-ray diffraction (XRD) methods. UV-Vis spectrum of synthesized silver nanoparticles from Mimosa pudica root powder extract shows a characteristic absorption peak at 421 nm. FTIR analysis reveals that presence of silver nanoparticles the presence of some biomolecules in extracts that act as reducing and capping agent for green synthesis of silver nanoparticles. DLS analysis showed AgNPs are drifted widely from 58.6 to 157.7 nm, with an average particle size of 104.7 nm. The particles are found to be polydisperse and slightly agglomerated due to the presence of phytochemicals present in the plant extract. Scanning electron microscope showed silver nanoparticles are spherical shaped. The XRD pattern revealed the presence of crystalline, dominantly spherical silver nanoparticles in the sample having size ranging from °, and 81.33°, 77.5°, 64.5°, 44.3° for leaves extract and 38.1°, and 77.32°, 64.42°, 44.22°42 to 50 nm. The XRD peaks 38.08 for callus extract can be assigned the plane of silver crystals (111), (200), (220), and (311), respectively, and shows facecentered, cubic and crystalline nature of the silver nanoparticles. The green synthesized silver nanoparticles show significant antibacterial activity.

Keywords: Antibacterial, FTIR, Mimosa pudica Root powder, Particle size, SEM, Silver nanoparticles, UV-Vis, XRD.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-030

INFLUENCE OF ZINC DOPING ON THE STRUCTURE, OPTICAL AND PHOTOCATALYTIC PROPERTIES OF ZN-DOPED $BATIO_3$ NANOCOMPOSITE

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ABSTRACT

In this study, a solid-phase technique aided by a sol-gel was used to manufacture of Zn-doped $BaTiO_3$ nanoparticles. To examine the structure and evolution of the resultant sample at various stages, a variety of instruments were used to conduct investigations, including X-ray diffraction (XRD), UV-Visible spectroscopy (UV), Energy dispersive X-ray spectroscopy (EDX), high resolution transmission electron microscopy (HR-TEM), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The growth and crystallization of Zn-doped $BaTiO_3$ were analyzed using XRD. Spherically shaped nanoparticles with minor aggregation and homogeneous size distribution are shown by SEM and HR-TEM investigations. Using UV-visible spectroscopy, the energy band structure and electron hole recombination of the samples were examined.

Keywords: Sol-gel Auto-combustion, Titanium dioxide, Zinc Nitrate, and morphology Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-031

INVESTIGATION ON EFFECT OF AG DOPING IN PHOTOCATALYTIC DYE DEGRADATION AND ANTIBACTERIAL ACTIVITIES OF A-CUV_2O_6 NANOPARTICLES

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ABSTRACT

Ag-doped α-CuV_2O_6 (Ag at 2, 4, and 6wt%) nanoparticles were synthesized through a hydrothermal-assisted co-precipitation method, followed by doping at varying weight percentages of 2, 4, and 6 wt%. The study examined how varying levels of doping affect the photocatalytic characteristics and antibacterial efficacy of the samples, revealing that the variation with 6 wt% doping exhibited the highest efficacy in both photocatalytic and antibacterial applications. X-ray diffraction analysis validated the triclinic structure of the synthesized Ag-doped α-CuV_2O_6 nanoparticles across the different doping levels. The mean crystallite size was calculated utilizing Scherrer's formula, was found to increase with higher doping percentages. The morphological characteristics of the nanoparticles were assessed using Scanning Electron Microscopy (SEM). Energy Dispersive Spectroscopy (EDS) confirmed the presence of Ag, Cu, V, and O in the synthesized nanoparticles. X-ray Photoelectron Spectroscopy (XPS) analysis revealed the existence of Ag, Cu, O, and V, with only trace amounts of absorbed carbon detected, thereby affirming the purity of the Ag-doped α-CuV_2O_6 phase, which exhibits a triclinic structure. UV-Visible spectrophotometry demonstrated a decrease in band gap values with increasing doping percentages. A significant peak in the photoluminescence (PL) emission spectra within the green wavelength range suggested the formation of deep energy levels in the

nanoparticles' band gap. The photocatalytic performance of the synthesized materials in degrading methylene blue dye under sunlight was evaluated using a UV-Visible spectrometer. The efficiency of degradation improved as the doping concentration increased, reaching its maximum at 6 wt%. The values escalated from 90.02 for 2wt% Ag to 96.20 for 6wt% Ag. The antibacterial properties of the synthesized compounds were assessed against Gram-negative bacterial strains, particularly Escherichia coli, resulting in noticeable zones of inhibition. The bacterial inhibition zones associated with Ag-doped α-CuV_2O_6 exhibited an increase from 4 mm at 2 wt% Ag to 16 mm at 6 wt% Ag. The nanoparticles with 6 wt% doping exhibited superior antibacterial activity, attributed to their significantly larger surface area, which enhances their effectiveness.

Keywords: Ag doped α-CuV_2O_6, Hydrothermal Co-precipitation, photocatalytic, degradation, Antibacterial activity.

National Seminar on Emerging Material Science Research (NSEMSR - 25)

(ISBN: 9789348505101)

A-032

STUDIES OF PURE TIO_2 AND BAO-LOADED TIO_2 NANOCOMPOSITES FROM STRUCTURAL, OPTICAL AND PHOTOCATALYTIC ACTIVITIES

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ABSTRACT

In this study, a solid-phase technique aided by a sol-gel was used to manufacture pure TiO_2, and 5wt% $BaTiO_3$ nanoparticles. To examine the structure and evolution of the resultant sample at various stages, a variety of instruments were used to conduct investigations, including X-ray diffraction (XRD), UV-Visible spectroscopy (UV), Energy dispersive X-ray spectroscopy (EDX), high resolution transmission electron microscopy (HR-TEM), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The growth and crystallization of pure TiO_2, and 5wt% $BaTiO_3$ were analyzed using XRD. Spherically shaped nanoparticles with minor aggregation and homogeneous size distribution are shown by SEM and HR-TEM investigations. Using UV-visible spectroscopy, the energy band structure and electron hole recombination of the samples were examined. The chemical and electronic states of the $BaTiO_3$ nanoparticles were identified using XPS analysis. The activity and selectivity of the photocatalytic process can be influenced by the arrangement of atoms on the crystal surface.

Keywords: XPS analysis, Sol-gel Auto-combustion, Titanium dioxide, Barium Titanate, and morphology Studies.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-033

GROWTH AND CHARACTERIZATION OF BARIUM NITRATE SINGLE CRYSTAL

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ABSTRACT

Inorganic Barium Nitrate (BN) crystals were grown by slow evaporation technique. Solubility of BN salt was 9 gm/100 ml good transparent crystals were grown after 4-5 weeks at ambient temperature. Structural analysis of grown crystals from powder XRD studies with unit cell parameter and volume. The grown crystals were characterized by powder X-ray diffraction, UV–visible spectroscopy, Fourier transform infrared spectroscopy (FTIR). The powder XRD study shows that the crystalline perfection of grown crystal is good. FTIR studies confirm the functional groups of the crystals. The UV-vis-NIR transmission studies show optical transparency in the entire visible region and has cut off wavelength is 239 nm. SHG efficiency has been studied by Kurtz Perry method.

Keywords: Crystal growth, optical Parameters, third order NLO.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-034

GROWTH AND CHARACTERIZATION OF THIRD ORDER NON-LINEAR PROPERTIES OF BARIUM NITRATE WITH NICOTINIC ACID SINGLE CRYSTAL

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ABSTRACT

Barium Nitrate with Nicotinic Acid single crystal was 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 UV-vis-NIR transmission studies show optical transparency in the entire visible region and has band gap energy is 5.09 eV. The third order nonlinear optical nature of BNAC single crystals was studied using Z – scan technique.

Keywords: Crystal growth, optical Parameters, third order NLO.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-035

RATIONAL DESIGN OF DENGUE VIRUS INHIBITORS: MOLECULAR DOCKING AND ADMET EVALUATION

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ABSTRACT

Dengue virus (DENV) is a significant global health threat, causing severe illnesses such as dengue fever, dengue hemorrhagic fever, and dengue shock syndrome. Despite its widespread impact, there is no specific antiviral treatment available, highlighting the urgent need for effective small-molecule inhibitors targeting key viral proteins. This study employs molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis to design and evaluate novel inhibitors against essential dengue virus proteins, including NS2B-NS3 protease and NS5 RNA-dependent RNA polymerase. Molecular docking simulations provide insights into binding interactions, hydrogen bonding networks, and hydrophobic contacts, identifying promising candidates with high affinity for the viral active sites. ADMET analysis predicts pharmacokinetic properties and toxicity profiles, ensuring optimal drug-likeness and safety. Additionally, structural insights into viral resistance mechanisms aid in the rational design of next-generation dengue antivirals. This integrated computational approach facilitates the development of potent and selective inhibitors, contributing to the advancement of dengue virus therapeutics.

Keywords: Dengue virus inhibitors, molecular docking, ADMET analysis, antiviral drug design, NS2B-NS3 protease, NS5 RNA-dependent RNA polymerase.

National Seminar on Emerging Material Science Research (NSEMSR - 25)

(ISBN: 9789348505101)

A-036

IN SILICO APPROACHES FOR ANTIFUNGAL DRUG DISCOVERY: MOLECULAR DOCKING AND ADMET EVALUATION

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ABSTRACT

Fungal infections pose a significant threat to human health, particularly in immunocompromised individuals. The increasing prevalence of antifungal resistance necessitates the development of novel inhibitors targeting key fungal enzymes and proteins. This study employs molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis to design and evaluate potential antifungal agents with improved efficacy and safety. Molecular docking simulations identify crucial binding interactions, hydrogen bonding networks, and hydrophobic contacts within fungal targets such as lanosterol 14α-demethylase and β-glucan synthase, which are essential for fungal cell membrane integrity. ADMET analysis predicts pharmacokinetic properties and toxicity profiles, ensuring optimal drug-likeness and minimal side effects. Additionally, structural insights into resistance mechanisms guide the rational design of next-generation antifungal inhibitors. This computational approach provides a foundation for developing potent and selective antifungal drugs, addressing the urgent need for effective antifungal therapies.

Keywords: Antifungal inhibitors, molecular docking, ADMET analysis, drug design, lanosterol 14α-demethylase, β-glucan synthase.

National Seminar on Emerging Material Science Research (NSEMSR - 25)

(ISBN: 9789348505101)

A-037

SOLVOTHERMAL SYNTHESIS OF [$SN_{1-X}MN_XS/BIVO_4$] COMPOSITE NANO PARTICLES OF PHOTO CATALYTIC PERFORMANCE FOR MB DEGRADATION

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ABSTRACT

In the present work successfully synthesized both undoped and manganese (Mn)-doped SnS/$BiVO_4$ composite nanoparticles (NPs) using a solvothermal method. This study focuses on the optical properties of SnS, $BiVO_4$, and Mn-doped SnS/ $BiVO_4$, analyzed through UV-visible absorption spectroscopy. The effect of Mn doping on the optical band gap of the SnS/$BiVO_4$ composite NPs was investigated, revealing that the optical band gap widens with different concentrations of Mn doping (2%, 4%, and 6%). Various characterization techniques, including X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM), were employed to confirm the XRD patterns of SnS and $BiVO_4$ has orthorhombic and tetragonal crystalline structure, binding energies and nano rod morphological features of the synthesized nanoparticles. The elemental status of SnS, $BiVO_4$, and Mn-doped SnS/ $BiVO_4$NPs was studied by EDAX. The enhanced photo catalytic activity can be attributed to Mn doping, which plays a significant role in lowering the band gap and increasing charge carriers, superoxide radicals, and hydroxyl radical production. A Z-scheme model is proposed to explain the charge transfer pathway in this system, highlighting its crucial role in enhancing the photo catalytic performance of the heterojunction.

Keywords: SnMnS/$BiVO_4$-nanocomposites; Solvothermal synthesis; HR-SEM; XPS; Photo catalyst applications.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-038

ARDUINO LED SOUND LEVEL METER USING MAX9814 AND 74HC595 SHIFT REGISTER

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ABSTRACT

In this work, we present the development and implementation of an LED Sound Level Meter utilizing the Arduino microcontroller platform. The primary objective is to design a compact and efficient system capable of providing a visual representation of ambient sound levels through a series of LEDs. Key components integrated into the system include the Arduino UNO for processing sound data, the MAX9814 microphone for accurate sound detection, and the 74HC595 shift register for effective LED management. This project aims to offer a practical tool for monitoring sound intensity in various environments, with potential applications in noise pollution assessment, audio engineering, and educational demonstrations.

The methodology involves converting sound waves into electrical signals via the MAX9814 microphone. These signals are processed by the Arduino, which determines the peak-to-peak sound levels. The shift register is employed to manage the LEDs, displaying different sound levels using a color-coded system: green LEDs for low sound levels, blue LEDs for medium levels, and red LEDs for high levels. The circuit design is meticulously crafted to ensure seamless integration of components, while the Arduino code is optimized for accurate and real-time sound level measurement.

Experimental results validate the system's performance, showcasing its capability to dynamically respond to varying sound intensities. The project also discusses calibration routines implemented to account for ambient noise variations, enhancing the precision of the measurements. The effectiveness of the LED Sound Level Meter is demonstrated through

practical applications, providing an accessible means for users to visualize and understand sound dynamics.

The project concludes with an evaluation of the system's strengths, including its cost-effectiveness and ease of implementation, while also identifying potential areas for improvement. Future work may explore the integration of wireless communication modules for remote monitoring, the addition of a digital display for numerical sound level readouts, and enhancements in microphone sensitivity for more detailed analysis.

In summary, this project successfully combines hardware and software components to create a functional and reliable LED Sound Level Meter, offering valuable insights into sound measurement and visualization techniques. The scope for further development and practical applications make this project a noteworthy contribution to the field of DIY electronics and educational tools.

National Seminar on Emerging Material Science Research (NSEMSR - 25)
(ISBN: 9789348505101)

A-039

STRUCTURE-BASED DESIGN OF COX INHIBITORS: MOLECULAR DOCKING AND ADMET ANALYSIS

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ABSTRACT

Cyclooxygenase (COX) enzymes, particularly COX-1 and COX-2, play a vital role in inflammation and pain regulation, making them key targets for anti-inflammatory drug development. However, the selectivity of inhibitors toward COX-2 over COX-1 is crucial to minimize gastrointestinal side effects while maintaining therapeutic efficacy. This study employs molecular docking and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis to design and evaluate novel COX inhibitors with improved selectivity and safety profiles. Molecular docking simulations provide insights into binding interactions, hydrogen bonding networks, and hydrophobic contacts within the COX active site, identifying structural features essential for potency. ADMET analysis further assesses pharmacokinetic and toxicity parameters, ensuring drug-likeness and reduced side effects. Structural insights into COX-2 selectivity mechanisms help guide the design of next-generation anti-inflammatory agents with enhanced therapeutic potential. This integrated computational approach aids in the rational design of potent and selective COX inhibitors, contributing to the development of safer and more effective anti-inflammatory drugs.

Keywords: COX inhibitors, molecular docking, ADMET analysis, anti-inflammatory agents.

About the University

Thiruvalluvar University was established by the Government of Tamilnadu in October 2002 under the Thiruvalluvar University Act, 2002 The University was inaugurated on 16 10 2002 as a State University The University is located in a Sprawling Campus of about 112 68 acres at the Serkkadu village which is on Ranipet Chittoor Trunk Road, 16 km away from the Vellore City The University named after the great Tamil Saint " The university has ten departments viz Physics, Chemistry, Mathematics, Biotechnology, Zoology, Computer Science, Economics, Commerce, Tamil and English There are 74 Arts and Science Colleges affiliated to this University.

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