VALLIAMMAI WOMEN'S COLLGE OF ARTS AND SCIENCE

(Affiliated to Annamalai University)

Near Arakandanallur, Villupuram District -605752, Tamil Nadu, INDIA

NATIONAL CONFERENCE ON RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE

(NCIRS-2026)

Date: 17-02-2026

Jointly organized by

DEPARTMENT OF PHYSICS, CHEMISTRY & MATHEMATICS

NATIONAL CONFERENCE ON RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE
(NCIRS-2026)

DATE: 17:02:2026

Conference Proceedings

CHIEF EDITORS & CONVENORS

Dr.R.Bomila,

Prof. R. Kavitha, Prof. K. Sathyapriya

VWC, Arakandanallur

Jointly organized by
Department of Physics, Chemistry and Mathematics
Valliammai Women's College of Arts and Science,
Near Arakandanallur,
Villupuram District - 605 752
Tamil Nadu, India.
2026

Title of the book	**:**	***NATIONAL CONFERENCE ON RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE***
Chief Editors	**:**	**Dr.R.Bomila,** **Prof. R.Kavitha, Prof K.Sathyapriya**
Organized by	**:**	**Department of Physics, Chemistry and Mathematics** **Valliammai Women's College of Arts and Science,** **Near Arakandanallur,** **Villupuram District - 605 752** **Tamil Nadu, India.**
First Edition	**:**	**2026**
Pages	**:**	**1 – 43**
ISBN	**:**	**978-81-996376-7-2**
Published	**:**	**Multi Spectrum Publications,** **No: 13/66, Thiruninarkurichy,** **Ammandivilai Post-629204,** **Kanyakumari, Tamilnadu, India**
Printed at	**:**	**Bala Computer, Chidambaram - 608002**

VALLIAMMAI WOMEN'S COLLEGE OF ARTS AND SCIENCE,
NEAR ARAKANDANALLUR, VILLUPURAM DISTRICT - 605 752

Chairman Message

The foundation stones of Valliammai Women's college of Arts and Science are laid on the essence of academic pursuit and excellence. Excellence in any work can be achieved with utmost dedication, hard work, and perseverance. We have made this dictum our motto and our way of life in every single activity in the campus.

Research and development forms the backbone of our curriculum in our Institution. The staff and students are engaged in various path-breaking innovative research activities all throughout the year. Every Department of our college organizes conferences and seminars frequently on contemporary and relevant topics in order to facilitate research in those areas which will lead to necessary metamorphosis in the academia as well.

It brings me immense pleasure to congratulate the Department of Physics, Chemistry & Mathematics on the successful organization of the conference **"RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE (NCIRS-2026)"** at Valliammai Women's College of Arts and Science, we believe in fostering a spirit of curiosity that goes beyond textbooks. This event is perfectly aligned with our mission to make scientific learning both experiential and innovative. I applaud the faculty for their dedication and the students for their enthusiastic participation. Such academic endeavors are crucial in shaping the next generation of scientists, engineers, and innovators.

The National Conference on **"RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE (NCIRS-2026)"** was jointly organized by the Convenor Dr.R.Bomila , Prof. R.Kavitha & Prof. K.Sathyapriya and other staff members of Department of Physics ,Chemistry and Mathematics. It is another venture to provide a platform for academicians –Professors, students, and research scholars nationally to discuss on contemporary trends and innovations in the subject of Chemistry.

I wish the conference all the very best and urge all participants to brainstorm on the various thrust areas of the conference. I also wish all of you a happy stay in our campus and look forward to your participation in various events in the campus.

Mr.V. Boopathy,M.A.,
Dy. Collector(Rtd)
Secretary/Chairman

VALLIAMMAI WOMEN'S COLLEGE OF ARTS AND SCIENCE,
NEAR ARAKANDANALLUR, VILLUPURAM DISTRICT - 605 752

Message By Principal

It is a matter of great pride and privilege to be a part of an esteemed organization Valliammai Women's college of Arts and Science that prepares today's students to meet the challenges of the Subject. I have seen the way our college has become pioneer in providing superior quality education in the neighboring areas and has also been engaged to extend these efforts further

This has become possible with the untiring efforts of our Department of Physics , Chemistry and Mathematics. They have organized one day National Conference on **"RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE (NCIRS-2026)"** which imparts research by relating it with real life scenarios and current developments in their respective fields. The Research topic is based on the ever changing needs of the subject .

As a Principal of Valliammai Women's college of Arts and Science, I am confident that efforts to excel in the field of higher education and the inculcation of moral values in the students at the Campus will continue in future with a greater zeal.

I, therefore Congratulate the Convenor of the Conference Dr. R.Bomila.,Head of, Department of Physics , Prof. R.Kavitha., Head of Department of Chemistry & Prof. K.Sathyapriya, Scholars, Head of Department of Mathematics, Staff and Students of the Physics & Chemistry department for the initiative of a National level Conference and wish the Department to be part of this revolution led by Valliammai Women's college of Arts and Science and become the stars of tomorrow.

Prof. N. Thennarasi ,
Principal

VALLIAMMAI WOMEN'S COLLEGE OF ARTS AND SCIENCE,
NEAR ARAKANDANALLUR, VILLUPURAM DISTRICT - 605 752

Message By Vice Principal

Francis Bacon said "Reading maketh a full man; conference a ready man; and writing an exact man". Conferences bring together people of varied experiences and provide an opportunity to everyone to share their thoughts. Mutual participation and high quality deliberations create inspiring learning environment resulting into innovative ideas. Today's industry expects such inputs to bring home new innovations and inventions.

We know that for students to compete internationally and become a part of the world they need to be creative and innovative. We cultivate in our students right attitude with blend of Conferences, seminars, extra-ordinary soft skills and hence make their personality impressive so that they become brand ambassadors of not only Valliammai Women's college of Arts and Science but also to the self. .

We as a team at Valliammai Women's college of Arts and Science strive to prepare students to become better citizens of our country irrespective of their cultural and financial background and contribute in the welfare of society and country's development.

I was absolutely delighted to witness the vibrant engagement at the recently concluded Physics , Chemistry & Mathematics **" RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE (NCIRS-2026)"** The event showcased the exceptional talent within our institution and brought complex, modern and scientific concepts to our doorstep.

A special note of appreciation to the entire Physics , Chemistry & Mathematics department for organizing this enlightening session. It is through such proactive academic initiatives that we bridge the gap between classroom theory and real-world applications.

Dr. S. Reena,
Vice Principal

ABOUT THE INSTITUTION

With a noble ambition to propagate women's education and with a sense of concern and commitment to the society at large, **VALLIAMMAI WOMEN'S COLLEGE OF ARTS AND SCIENCE** was started during 2010-2011 by the Philanthropic minded trustee of VALLIAMMAI EDUCATIONAL AND CHARITABLE TRUST, Chidambaram. The college aims at serving for improvement of the standard of women in Tamilnadu with the help of education. This women's college in the rural area in Villupuram district provides life oriented education along with job avenues, results in the generation of enlightened women with abundant force of aspiration and ambition suitable in accordance with the realities of life.

Vision:

To mould every individual student who leaves its portals into a human, socially responsible and professionally successful woman who can envision her strive towards perfection without compromising on the ethical values.

Mission:

To help young students grow into a confident, creative, emotionally balanced and potentially competent woman by nurturing their all-round potential through an excellent educational system.

ABOUT THE DEPARTMENT

Department of Physics:

The Department of Physics & Chemistry was established in the year 2011 with B.Sc. and 2018 with M.Sc. Physics & Chemistry. It is well equipped to support high quality teaching and laboratories for both UG & PG students separately with standard activities. It has qualified and dedicated faculty to give the lecture effectively and guide the students in the right way.

Department of Chemistry:

The Department of Chemistry was established in the year 2011 with B.Sc., Chemistry and 2018 with M.Sc., Chemistry as a new Science Department with an objective of providing quality education in the conventional areas of Science and growing into a center for teaching and research with an aim to acquire prominent position in the academic map.

Department of Mathematics:

The Department of Mathematics was established in the year 2010 with B.Sc., Mathematics and & in 2018 with M.Sc Mathematics . To provide a strong mathematical foundation through innovative and comprehensive curricula, tailored to meet the unique needs of various academic disciplines to empower students with critical thinking, quantitative reasoning and computational skills, preparing them for successful careers in academic, industry and research.

OBJECTIVES OF THE CONFERENCE

National Conference on "Recent trends in Interdisciplinary Research in Science" **(NCIRS-26)** invites all researchers working the dynamic convergence of these sciences and foster innovative solutions to contemporary challenges. It serves as a vital platform for researchers, academicians, industries and students to exchange groundbreaking ideas, bridging traditional academic boundaries. To bring out the recent innovation in Physics, Chemistry & Mathematics from the young researchers will be the highlight of this conference.

The Conference will cover the following Areas.

PHYSICS: Crystals Growth & Application, Nanomaterial, Techonology & Application, Medical Physicscs, Solar cell Application Advanced Material Science, Spectroscopy, Crystallography, Non-lineal optics.

CHEMISTRY: Inorganic Chemistry, Organic Chemistry, Electrochemistry, Analytical Chemistry, Pharmaceutical Chemistry, Environmental Chemistry, Polymer Compounds, Catalysis,Spectroscopy,Green Chemistry.

MATHEMATCIS: Mathematical Modeling, Algebra & Analysis, Cyber security, Soft computing , Fizzy, Meural, crenetic Algorithms., Biostatistics., Statistics & Data science, Applied statics, Internet of things.

Organizing Committee

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Dy. Collector (R)**,** Chairman/Secretary
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Valliammai Women's College of Arts & Science,
Arakandanallur-605752

Dr. S. Reena,
Vice Principal
Valliammai Women's College of Arts & Science,
Arakandanallur-605752

Eminent Speakers

Dr. S.Srinivasan
Associate Professor,
PG & Research Department of Physics
Presidency College (Autonomous)
Chennai.
Title: Design and Evaluation of efficiency of the Solar Cell by using SCAPS1D software

Dr. R. Arulraj
Professor,
Centre for Research and Development
Sri Manakula Vinayagar Engineering College,
Puducherry.
Title:"Conducting Interdisciplinary Research and Communicating High-Impact Journal Publications"

Dr .P. Kandan,
Assistant Professor
Department of Mathematics
Annamalai University
(On Deputation to Govt. Arts College, Chidambaram)
Title: The Impact of Mathematics across diverse fields

CONVENOR

Dr. R. Bomila,
Assistant Professor & Head
Department of Physics,
Valliammai Women's College of Arts & Science,
Arakandanallur-605752.

Prof. R. Kavitha, M.Phil.,
Assistant Professor & Head
Department of Chemistry,
Valliammai Women's College of Arts & Science,
Arakandanallur-605752.

Prof. K.Sathyapriya,
Assistant Professor & Head
Department of Mathematics,
Valliammai Women's College of Arts & Science,
Arakandanallur-605752.

COMMITTEE MEMBERS

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VALLIAMMAI WOMEN'S COLLEGE OF ARTS AND SCIENCE,
NEAR ARAKANDANALLUR, VILLUPURAM DISTRICT - 605 752

UG COURSES OFFERED	PG COURSES OFFERED
B.A., TAMIL	M.A., TAMIL
B.A., ENGLISH	M.A., ENGLISH
B.B.A.,	M.Sc., PHYSICS
B.Sc., MATHEMATICS	M.Sc., CHEMISTRY
B.Sc., PHYSICS	M.Sc., MATHEMATICS
B.Sc., CHEMISTRY	M.Sc., COM.SCIENCE
B.Sc., COM.SCIENCE	M.COM
B.C.A.,	M.Sc., MICROBIOLOGY
B.COM., (CA)	
B.COM.,(GENERAL)	
B.Sc., MICROBIOLOGY	

NATIONAL CONFERENCE ON "RECENT TRENDS IN INTERDISCIPLINARY RESEARCH IN SCIENCE (NCIRS-2026)"

PROGRAMME SCHEDULE

DATE: 17:02:2026 **VENUE: AUDITORIUM**

TIME	:	EVENT
9.00 AM -9.30 AM	:	REGISTRATION
9.30 AM-10.15 AM	:	INAUGURATION
TECHNICAL SESSION		
SESSION I: 10.15 AM -11.30 AM Design and Evaluation of efficiency of the Solar Cell by using SCAPS1D software	:	**Dr. S.Srinivasan** Associate Professor, PG & Research Department of Physics Presidency College (Autonomous) Chennai.
11.30AM -11.50 AM	:	TEA BREAK
SESSION II: 11.50 AM – 12.40 PM Conducting Interdisciplinary Research and Communicating High-Impact Journal Publications	:	**Dr. R. Arulraj , Professor,** Centre for Research and Development Sri Manakula Vinayagar Engineering College, Puducherry.
12.40 AM -1.15 PM	:	POSTER PRESENTATION
1.15 PM - 2.00 PM	:	LUNCH BREAK
SESSION III: 2.00PM-2.45PM The Impact of Mathematics across diverse fields	:	**Dr .P. Kandan,** Assistant Professor Department of Mathematics Annamalai University (On Deputation to Govt. Arts College, Chidambaram)
2.45 PM-3.15 PM	:	PAPER PRESENTATION
3.15 PM-3.30 PM	:	VALEDICTION

Design and Evaluation of efficiency of the Solar Cell by using SCAPS1D software

Dr.S. Srinivasan [a]*

[a]*Department of Physics, Presidency College (Autonomous), University of Madras, Chennai 600005, TN, India*

Solar cells generate electricity without producing greenhouse gas emissions during operation, making them crucial for reducing carbon emissions and combating climate change. Unlike fossil fuels, they don't pollute the air or water, helping to preserve ecosystems and improve public health.Sunlight is essentially unlimited on human timescales. Unlike coal, oil, or natural gas which will eventually run out, solar energy is renewable and will be available for billions of years.SCAPS-1D (Solar Cell Capacitance Simulator in 1 Dimension) is a widely-used software tool for solar cell research and development.SCAPS-1D simulates the electrical characteristics of thin-film solar cells by solving fundamental semiconductor equations (Poisson's equation and carrier continuity equations). It helps researchers predict how solar cells will perform without needing to physically fabricate every design variation. A detailed analysis has been carried out on changing the different physical parameters for obtaining the optimization condition was done to compute the power conversion efficiency (PCE) of the solar cell. The obtained results were analyzed. Simulation result opens new avenue for green energy electricity at low cost with environment-friendly materials as component of the solar cell.

Conducting Interdisciplinary Research and Communicating High-Impact Journal Publications

Dr. R. Arulraj[a]

[a]*Centre for Research and Development, Sri Manakula Vinayagar Engineering College, Puducherry.*

Interdisciplinary research is crucial in addressing complex scientific, technical, and societal issues that transcend traditional academic boundaries. This presentation provides an organized and practical guide for academics on how to undertake multidisciplinary research and successfully publish in high-impact journals. The session opens by defining the core aim of research, highlighting its contribution to knowledge development, innovation, and the resolution of real-world problems in the scientific, industrial, environmental, and medical domains. Key concepts of multidisciplinary research are explored, emphasizing their significance in generating innovation and increasing citation impact. The presentation methodically discusses key components of research technique, such as problem identification, literature review, research design, data collection, analysis, and validation, using examples from scientific, applied, and translational research. The emphasis is on repeatability, ethical research techniques, and the appropriate use of analytical and statistical tools. Furthermore, the structure and best practices for scientific writing are discussed, including manuscript organization, clarity, plagiarism avoidance, and strategic journal selection. The journal submission and peer-review procedure are also reviewed, with tips on how to respond to reviewer remarks and ensure ethical compliance. The talk concludes by discussing larger opportunities for scientific communication, including conferences, patents, and public participation. Overall, the goal of this session is to provide researchers with the tools they need to conduct effective multidisciplinary research and publish their findings successfully.

Keywords: Interdisciplinary research; Research methodology; Scientific writing; Journal publication; Peer review; Research communication

The Impact of Mathematics in Diverse Fields

Dr.P.Kandan[a*]
[a]Department of Mathematics, Annamalai University ,Government Arts College, Chidambaram

Mathematics functions as a universal language that enables the understanding, modeling, and analysis of structures and relationships across diverse disciplines. This talk titled "The Impact of Mathematics in Diverse Fields" highlights the fundamental role of mathematics—particularly graph theory, matrix theory, and allied concepts—in addressing real-world problems in science, engineering, technology, and social systems. Mathematical reasoning allows complex and interconnected phenomena to be transformed into structured models that can be systematically analyzed, optimized, and interpreted.Similarly, abstract systems like social networks, biological systems, computer networks, and the World Wide Web display intricate patterns of connectivity. Graph theory provides a powerful mathematical framework to represent such systems using vertices and edges, facilitating visualization and analysis. This lecture introduces essential graph-theoretic concepts including vertices, edges, walks, paths, and directed graphs. Directed graphs are especially useful for modeling systems where direction plays a critical role, such as traffic flow, project scheduling, information transfer, and social media interactions. Mathematical principles like the Handshaking. Hypercube graphs have applications in computer architecture and molecular biology. The interdisciplinary impact of mathematics extends to chemistry, molecular biology, electrical engineering, artificial intelligence, and software testing. Graph-based models simplify molecular structures, support intelligent systems, and improve software reliability. Beyond discrete mathematics, numerical analysis and differential equations model continuous phenomena such as population growth, heat transfer, and mechanical motion. Overall, mathematics emerges as a unifying and practical discipline that bridges theory and application, supports innovation, and enhances our ability to understand and manage complex real-world systems.

Synthesis of Silver Nanoparticles Using Tomato Extract as Stabilizing Agent and their Characterization

R. Kavitha[a*]
[a]Department of Chemistry, Valliammai women's college of arts and science, Arakandanallur*

Silver nanoparticles had drawn the attention of researcher due to its biological activity. An eco-friendly method using *Tomato* extract as a source of effective reducing agent was reported to prepare Silver nanoparticles (Ag NPs). Biosynthesized AgNPs were characterized by UV-Visible, FTIR, XRD and TEM techniques. The stretching frequency of Ag NPs and absorption maximum were confirmed by FTIR and UV-Visible spectra. TEM morphology study showed various shapes of nanoparticles, and hence it can be used as biomaterials for the development of antibacterial agent.

Keywords: Silver nanoparticles, Tomato extract, Morphology study, Characterization activity

Green Synthesis of CeO_2-NPs Using Datura Stramoniu Leaf Extract and their Antibacterial Activities

Dr.R.Bomila[a] , Dr.S.Srinivasan[a*], Dr. A.Muthuvel[b]

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[a] Department of Physics, Presidency College (Autonomous), University of Madras, Chennai 600005, TN, India*
[b]Department of Physics, DR.R.K.Shanmugam College of arts and science college (affiliated to Annamalai University, Chidambaram), Kallakurichi, Tamil Nadu – 606213, India

Cerium oxide nanoparticles (CeO_2-NPs) have been biosynthesized using the *Datura stramoniu* aqueous leaf extract, Biosynthesized particles have been characterized through the use of Structural properties (XRD), Optical properties (UV-Vis, Band gap, PL) in further, antibacterial activity. The diffraction peaks in the XRD spectrum of biosynthesis CeO_2-NPs occurring at 2θ values of 32°, 40°, 64°, 80° and 84°are indexed as the (110), (200), (220), (311) and (222) crystal planes face centred cubic structure. The absorption spectra of pure and biosynthesis CeO_2-NPs nanoparticles were analyzed in the UV-Vis spectra of pure and *A. Indica*leaf extract (5 and 10 ml) using biosynthesis CeO_2-NPs. The absorption peaks locate at 271, 268 and 264 nm pure and biosynthesis CeO_2-NPs respectively. A distinct blue shift is observed in the absorption of 10 ml leaf extract as compared to the pure and other concentration solution. The appearance of three different peaks with Gaussian Function was achieved for all the PL spectra. The Near band edge emission observed at 392, 448 and 467 nm for pure and biosynthesis CeO_2-NPs respectively. In studied PL of 3D-flower like CeO2-NPs prepared by biosynthesis method. The strongest peak at ~392 nm was attributed to the 5d →2 F5/2 and 5d→ 2 F7/2 respectively. the different inhibition zones for CeO_2 NPs on bacillus subtitles (12 mm) and E. coli (17 mm) strains. We observed that high zone of inhibition of biosynthesis CeO_2 NPs using *A.Indica*leaf extract (10 ml) for E. coli when compared with bacillus subtitles. This result clearly confirmed that antibacterial action of the biosynthesized CeO_2-NPs is fairly higher on E. coli than on bacillus subtilies.

Keywords: XRD, UV-Vis, PL, Antibacterial Studies, E.Coil, Datura stramoniu

Extremal and Probabilistic Techniques in Modern Graph Theory

K. Sathyapriya[a*]

[a]Department of Mathematics, Valliammai women's college of arts and science, Arakandanallur*

Extremal and probabilistic graph theory study the size and structure of graphs under given constraints and the role of randomness in graph properties. This project focuses on extremal problems such as Turan-type and Ramsey results, using probabilistic methods and random graph models. It also examines threshold behavior and stability in random graphs, highlighting the interaction between deterministic and probabilistic techniques. The study aims to obtain improved bounds and structural insights with applications to network analysis and combinatorial optimization.

Keywords: Extremal, probabilistic, modern

Expert Opinion Fuzzy Fusion (EOFF) Method and its application: Freedom to Decision Makers

Stephen Mariadosa [a*], ***Felix Augustin*** [a]

[a*], *Rajalakshmi Institute of Technology, Chennai, Tamil Nadu, India.*

[a]*Department of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Chennai-600127, Tamil Nadu, India.*

Multi Criteria Decision Making (MCDM) methods are widely applied across diverse disciplines, and many have been enhanced with fuzzy logic to better address real-world problems characterized by uncertainty or linguistically expressed data rather than precise numerical values. In conventional fuzzy MCDM approaches, decision makers are typically restricted to a single fuzzy scale, limiting their flexibility in constructing the decision matrix. To address this, the present work proposes a fuzzy MCDM model that grants decision makers the freedom to select from multiple fuzzy scales, including triangular, trapezoidal, pentagonal, hexagonal and heptagonal fuzzy numbers. An alpha-cut aggregation method is introduced to combine decision matrices, and a closed-form center of gravity defuzzification technique is developed specifically for trapezoidal fuzzy numbers. The proposed method is validated through a case study on medical waste treatment, with its effectiveness further demonstrated via comparative and sensitivity analyses.

Keywords: Fuzzy MCDM, Poly fuzzy scales, Alpha-cut aggregation, Centre of Gravity defuzzification, Medical waste treatment

Spectroscopic and Quantum Chemical Analysis of Acetic Acid, Cyclohexyl Ester

L. Akalya [a], ***Dr.R.Bomila*** [a*]

[a,,a*]*Department of Physics,Valliammai Women's College of Arts and Science, Arakandanalur605752*

Acetic acid, cyclohexyl ester (cyclohexyl acetate) was characterized using Gas Chromatography–Mass Spectrometry (GC–MS), Fourier Transform Infrared (FT-IR) spectroscopy, and frontier molecular orbital (HOMO–LUMO) analysis to investigate its structural, spectroscopic, and electronic properties. The GC–MS analysis confirms the molecular identity and purity of the compound through its molecular ion peak and characteristic fragmentation pattern, supporting the proposed molecular formula. The HOMO–LUMO analysis, performed using Density Functional Theory (DFT), reveals that the HOMO is mainly localized over the oxygen atoms and cyclohexyl moiety, whereas the LUMO is predominantly concentrated on the carbonyl group, indicating possible intramolecular charge transfer. The calculated HOMO–LUMO energy gap suggests good molecular stability and low chemical reactivity**.**

Keywords: FT-IR, DFT, Cyclohexyl Ester

Influence of nature deep eutectic solvents on the electronic structure and photocatalytic dynamics of ZnO nanoparticles

A. Muthuvel[a*], V.Mohana[a]

[1]Department of Physics, DR.R.K.Shanmugam College of arts and science college, Chidambaram, Kallakurichi, Tamil Nadu – 606213, India

[2]Department of Physics, Government Arts and science college, Kallakurichi, Tamil Nadu – 606213, India

In this study, zinc oxide nanoparticles were facial prepared using DES – deep eutectic solvent mixture and their dye degradation potential towards Methyl blue and Methylene red was investigated. Their physiochemical attributes of prepared material were examined. Structural findings reported that the ZnO exhibited a hexagonal wurtzite crystallization with decreases on their crystallite size via DES incorporation. XPS examination indicated the Zn^{2+} presence, lattice oxygen, and surface hydroxyl groups on the ZnOnano catalyst. Morphological results combined with EDX were confirmed that the nanoparticles exhibited a spherical shaped uniform particle dispersion, with elemental purity. Optical analysis indicated that the blue shift was observed in ZnO absorption edge with the increased optical band gap to 3.5 eV. The FTIR detected Zn – O bonds as well as organic and hydroxyl groups derived from DES, which facilitate charge carrier mobility. Photoluminescence (PL) analysis indicated that oxygen vacancies played a role in suppressing electron – hole recombination. The BET surface area analysis revealed a porous structure favourable for photocatalytic reactions. The photocatalysis properties for the degradation of Methyl blue and methylene red were improved with DES and showed maximum degradation percentage 99 % and 97 % for DES - ZnO nanoparticles. The improved results are attributed to the increased charge carrier concentration induced by DES, which restricts the electron – hole recombination rate. Overall, the DES assisted ZnO nanoparticles demonstrated superior photocatalytic performance due to their reduced crystallite size, modified surface chemistry, increased surface area and improved charge separation making them promising candidates for environmental remediation applications.

Keywords: ZnO nanoparticles, DES, XPS, BET, Photocatalytic

Combined Spectroscopic and Frontier Orbital Analysis of 1-Piperidinepropanoic Acid with Potential Energy Distribution (PED)

G. Anitha[a], Dr. R. Bomila[a*]

[a,a]Department of Physics, Valliammai Women's College of Arts and Science, Arakandanalur-605752*

1-Piperidinepropanoic acid was investigated through a combined spectroscopic and theoretical approach to elucidate its structural, vibrational, and electronic properties. Density Functional Theory (DFT) calculations were employed to optimize the molecular geometry and support the experimental vibrational assignments. A detailed Potential Energy Distribution (PED) analysis was performed to accurately correlate the calculated normal modes with experimental FT-IR bands, enabling reliable assignment of fundamental vibrations. The HOMO–LUMO analysis reveals that the HOMO is mainly localized over the piperidine nitrogen and adjacent carbon framework, while the LUMO is concentrated over the carboxyl group, indicating possible intramolecular charge transfer. The computed HOMO–LUMO energy gap suggests good molecular stability with moderate chemical reactivity.

Studies on the action of mercapto azole additives on the coating and bath characteristics of autocatalytic copper nano film deposition

S. Absara Fdo[a*], P. BalaRamesh[b] and P. Venkatesh[c]

[a]Department of Chemistry, Vels Institute of Science, Technology and Advanced Studies, Chennai.*

[b] Department of Chemistry, R.M.K. Engineering College.

[c] Department of Chemistry, Pachaiyappa's College, Chennai.

This article aims at analyzing the influence of structurally related two azole additives such as 2-Mercaptobenzothiazole (2-MBT) and 2-Mercaptobenzimidazole (2-MBI) in the rate of autocatalytic copper nano film depositions. The effect of these stabilizers on the characteristics of both the electroless plating bath and electroless copper deposition is also studied. Dimethylamine borane (DMAB) is employed as the reducing agent and sorbitol as complexing agent in the copper methanesulphonate bath. Potassium hydroxide acts as the suitable pH regulator to modify the properties of copper nano deposits. 1 ppm of the azole additives are added in this eco-friendly bath and optimized at a pH of 12.75 ± 0.25 at a temperature of 28±2 ℃. The results obtained from various studies imply that 2-MBT had an inhibiting effect on copper deposition, whereas 2-MBI accelerated the deposition rate. The physical properties like deposition rate, thickness and activation energy are calculated to support the stabilizing effects of 2-MBT and 2-MBI. Surface morphology of the copper deposits is characterized by Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) techniques. Structural properties such as crystallite size and specific surface area of plain bath and additives laden baths are investigated using X-ray diffraction studies.

Keywords: 2-mercaptobenzimidazole, 2-mercaptobenzothiazole, dimethylamine borane, sorbitol, surface morphology

In Silico Investigation of Azine Derivatives as potential Antibacterial Agents Using DFT

S.Rajapriya[a] and R. Arulmani [a*]

[a,a]PG & Research Department of Chemistry, Govt. Arts College, C. Mutlur, Chidambaram*

Unsymmetrical Azine derivatives have shown promise as antibacterial agents. In this study, Density Functional Theory (DFT) Calculations using B3LYP/6-31G were performed to investigate the molecular structure and properties of Unsymmetrical Azine derivatives. The optimized geometries, vibrational frequencies, and electronic properties were analyzed to identify potential antibacterial activity. Molecular docking studies were also conducted to evaluate binding affinity with bacterial targets. The results sugget that Unsymmetrical Azine derivatives exhibit potential antibacterial activity, with specific compounds showing promising binding energies. This study provides insights into the design and development of novel Unsymmetrical Azine – based antibacterial agents.

Keywords: Unsymmetrical azine, silico method, Antibacterial.

Synthesis of nickel oxide nanoparticles using plant leaf extract of their antibacterial, and anti-oxidant activity

ManogarPriya[a]*, JawaharSukumaran[a]
[a,a*] *Department of Chemistry, School of Basic Sciences, VISTAS, Chennai 600117, Tamil Nadu, India*

This present work employed a straightforward, green synthesis methods to produce nickel oxide nanoparticles (NiONPs) utilizing the leaf extract from the green plant. The synthesized NPs underwent thorough characterization methods with UV-Visible spectroscopy (UV-Vis), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDAX), and transmission electron microscopy (TEM) analysis indicated the NiO NPs were predominantly monoclinic, cubic and hexagonal in shape, exhibiting high purity, has a general crystalline size ranging from 25 to 10 nm. Green-synthesised NiO NPs exhibited excellent 1,1-diphenyl-2-picryl hydrazyl (DPPH) free radical scavenging activity and interesting antibacterial activity against gram-positive and gram-negative bacteria. Notably, the results indicated that the extract from plants can produce NiO NPs with promising effects for use in the field of biological applications.

Keywords: Green synthesis;Plant Extract; NiO NPs; antibacterial; anti-oxidant

GC–MS, FT-IR and DFT Based HOMO–LUMO Studies on 2-Propenamide, N-(1-cyclohexylethyl)

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2-Propenamide, N-(1-cyclohexylethyl)- was investigated using Gas Chromatography–Mass Spectrometry (GC–MS), Fourier Transform Infrared (FT-IR) spectroscopy, and Density Functional Theory (DFT) based HOMO–LUMO analysis to elucidate its structural, spectroscopic, and electronic properties. The GC–MS analysis confirms the molecular identity of the compound through its molecular ion peak and characteristic fragmentation pattern, supporting the proposed molecular formula and purity. The HOMO–LUMO analysis, performed using DFT calculations, reveals that the HOMO is mainly localized over the amide nitrogen and adjacent unsaturated propenamide moiety, whereas the LUMO is predominantly distributed over the carbonyl group, indicating possible intramolecular charge transfer within the molecule.

Structural, Optical And Morphological Properties Of Pure And PEG Doped CdO Nanoparticles

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The synthesized particles were characterized using various techniques. The UV-vis spectrophotometer was used to measure the excitation and band gap of the samples. The presence of different functionalities on the capping agents and their retention on nanoparticle functionalization could be characterized by Fourier transform infra-red spectrometer (FT-IR). Nano crystals of Pure and PEG doped (2%, 4%, and 6%) CdO nanoparticles have successfully synthesized via the chemical precipitation method. In this an easy and cast effective technique for synthesis of nanoparticles in a large scale and studied for their, structural, functional, optical, and morphological properties. XRD study confirmed the particles sizes ranging from 34 to 29 nm. FT-IR study confirmed the metal oxygen (CdO) vibrations at 437, 457, 454, 451, 511 and 651 cm^{-1}. Further, the band gaps were identified by UV-Vis spectroscopy and the morphological analysis shows the crystalline sizes were decreased with increasing the doping constant compare to pure CdO nanoparticles. Therefore, the present study has been useful and helpful for the applications for various semiconductors and industrial fields.

Keywords: UV-Vis, FT-IR, CdO, PFG

A Fuzzy Set Fleet Administration Management System

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This paper surveys the contributions and application of fuzzy set in the area of fleet administration management system. A Fuzzy set fleet administration management system is software solution that leverages fuzzy logic and set theory to optimise and manage fleet operations , such as vehicle allocation ,routing and maintenance scheduling , by handling uncertain or imprecise data and making decisions based on vague criteria. Fleet management software (e.g., Fleetio, Keep Truckin),Route optimization tools (e.g., Route XL, Workwave) ,AI-powered transportation management system, Vehicle telematics platforms (e.g., Fleetio, Omnitracs),GPS and IoT for real -time tracking .

Keywords: AI, GPS, Telematics, Route XL.

Green Fabrication of Zinc Oxide Nanoparticles from Lawsonia inermis and Assessment of Their Germination Potential

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Green synthesis has attracted considerable attention as a reliable, sustainable, and eco-friendly approach for the production of a wide range of nanomaterials, including metal oxide nanoparticles, hybrid materials, and bio-inspired structures. This approach is increasingly recognized as an effective alternative to conventional synthesis methods, which often rely on hazardous chemicals and generate toxic byproducts. In particular, the biological synthesis of zinc oxide (ZnO) nanoparticles has emerged as a promising substitute for traditional chemical routes, significantly reducing associated environmental and health risks.In the present study, Lawsonia inermis (henna) leaf extract was utilized for the green synthesis of ZnO nanoparticles using the sol–gel method. The synthesized nanoparticles were subsequently evaluated for their effects on mung bean (Vigna radiata) seed germination. The results revealed notable influences on germination percentage as well as early seedling growth, highlighting the potential agricultural applications of biogenically synthesized ZnO nanoparticles.

Keywords: Lawsonia inermis, Zinc oxide nanoparticles, Green synthesis, Eco-friendly approach, Metal oxides, Seed germination.

Synthesis and functional material of 2,6-DIMETHYL-7-OCTEN-3-OL

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2,6-Dimethyl-7-octen-3-ol was investigated using a combination of spectroscopic techniques and theoretical optimization studies to elucidate its structural, vibrational, and electronic properties. The FT-IR spectrum exhibits a broad absorption band in the region 3400–3300 cm^{-1}, attributed to the O–H stretching vibration of the hydroxyl group, indicating the presence of hydrogen bonding. The combined spectroscopic and optimized theoretical analyses provide a comprehensive understanding of the molecular structure and electronic behavior of 2,6-dimethyl-7-octen-3-ol, highlighting its relevance in flavor and fragrance formulations, organic synthesis, and functional material studies.

A Study on Phytochemical Screening and Antibacterial Potential of Pomegranate, Papaya and Potato Peel Extract

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Plants are wealthy sources of antimicrobial agents as they contain a different variety of phytoconstituents. These types of natural drugs are always a better substitute of synthetic drugs. This study investigated the qualitative screening of phytochemicals from pomegranate, papaya, potato peel using polar and non-polar solvent and in vitro antibacterial activity of these peel extracts. The data presented here indicate that the peel of pomegranate was produced effective against both Gram-positive and Gram-negative bacteria compared to potato and papaya peel. Gram-negative bacteria were found to be more sensitive towards all extract than the Gram-positive ones. Among the solvents, aqueous polar solvent was found to be more significant than the chloroform non-polar solvent against the test strains. This may be the presence of maximum number of phytochemicals present in aqueous extract. The results predict that the polar solvent extract of these peels can be used as natural antibacterial agent to cure human diseases.

Keywords: Pomegranate, Papaya, Potato, Peel extract, Phtochemicals, Antibacterial**.**

The Soret Effect on Free Convective Unsteady MHD Flow Over a Vertical Porous Plate With a Heat Source in Uniform Porous Medium

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This study investigates the soret effect on unsteady magnetohydrodynamic (MHD) free convective flow of a viscous, incompressible ,and electrically conducting fluid past a vertical porous plate, with a heat source within a porous medium.The governing equations, considering thermal diffusion, heat generation, and a transverse magnetic field, are solved using perturbation techniques. Results indicate that increasing the soret number (thermal diffusion) enhances velocity, concentration, and temperature fields. Increasing the magnetic field (M) and Prandtl number (Pr) tends to reduce velocity and temperature, while heat source parameters often enhance flow velocity.

Keywords: Soret Effect, MHD Parameter, Heat Source, Porous Medium

Synthesis and characterization of phosphonium based ionic liquids for mild steel corrosion in 1M HCl medium

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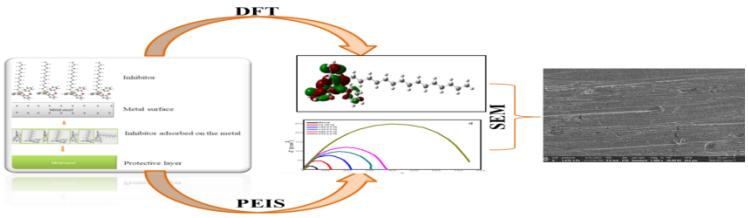
Graphical



The inhibition performances of three phosphonium containing ionic liquids with variable alkyl chain length namely, butyl triphenyl phosphonium bromide (BTPB), hexyl triphenyl phosphonium bromide (HTPPB) and hexadecyl triphenylphosphonium bromide (HDTPPB) were synthesized and their mild steel inhibition effect in 1M HCl was evaluated by weight loss method, potentiodynamic polarization studies, electrochemical impedance spectroscopy, SEM and quantum studies (DFT). Hence, theoretical calculations were used to explore the inhibition mechanism. The results showed that HDTPPB has 97% of grater inhibition than BTPPB and HTPPB. Adsorption studies obey the Langmuir isotherm. SEM results supported the protective layer formed on the mild steel. Furtheremore, increasing the alkyl chain length in ionic liquids could increase their inhibition efficiency.

Keywords: Mild steel, Ionic liquids, Adsorption, SEM, Inhibitor.

Simulation on Queuing Theory in Personnel Management

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Queuing theory can be predict some of the important parameters like total weighting time, average waiting time of patients, average queue length. The simulation of queuing system can be applied to personnel management pharmacy is the last department for out patient in hospital, the efficiency of which is directly associated with patient satisfaction and reputation of the entire hospital. The aim of the study is to improve the efficiency of queuing system of pharmacy base on queuing simulation method. After simulating suitable models for the current situation them improve the queues, there would be more profits made and moetmetme to carry out business than ever before, which would be very useful in this fast faced world. This results shows that and using their single server single queuing model to calculate the weighting time to patients

A Comparative Study of the Surface Morphology of an Electroless Copper Deposition Bath using a Green and a Non-Green Solvent

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This article reports the comparative study of surface morphology of the copper deposits using a green and a non-green solvent in an electroless copper deposition bath. The electroless copper plating was studied electrochemically using polyhydroxylic alcohol, Glycerol as the complexing agent and the reducing agents used are, a green solvent, Dimethylamine borane (DMAB) and anon-green solvent formaldehyde. The pH of the copper methane sulphonate bath was maintained by using Potassium hydroxide as the pH adjuster.The copper electroless bath was optimized by adding stabilizers at a concentration of 1ppm at 11.50 ± 0.25 pH for DMAB and at 13.0 ± 0.25 pH for HCHO. Alanine and Phenyl alanine are used as stabilizers. Their effects on plating bath were studied and reported. The characterization (SEM, AFM, XRD and CV studies) shows that the deposition using DMAB contained bath showed better and eco-friendly results than the formaldehyde used deposition bath.

Keywords: Glycerol, Dimethylamineborane, Formaldehyde, Alanine, Phenylalanine.

Synthesis and spectral analysis of some novel Pyridine Based Aryl Imines

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A series of novelpyridine-substituted heterocyclic Schiff bases were successfully synthesized via a condensation reaction between aromatic pyridine-carboxaldehyde derivatives and various primary amines bearing heterocyclic moieties (e.g., imidazole, thiazole, pyrazole, or triazole). The synthesis was carried out under mild catalytic or solvent-free conditions, yielding the target compounds with good efficiency. The structural elucidation of all newly synthesized compounds was performed using comprehensive spectral analysis.Fourier Transform Infrared (FT-IR)spectroscopy confirmed the formation of the characteristic azomethine (C=N) linkage, evident by a sharp band in the region of 1600-1650 cm^{-1}.Nuclear Magnetic Resonance (^{1}H & ^{13}C NMR) spectroscopy provided detailed evidence of the molecular framework, revealing the imine proton resonance (δ 8.0-8.5 ppm) and the distinct signals for the pyridine and other heterocyclic ring protons and carbons. Further confirmation of the molecular ion peak and purity was obtained throughMass Spectrometry (MS). These compounds are of significant interest as potential ligands for coordination chemistry and as promisingscaffoldsforfurtherpharmacologicalevaluationduetotheknownbioactivityofboth pyridine and Schiff base motifs.

Keywords: Schiffbase Ligands ;Heterocyclic Compound; conformations; bioactivity.

Structural, Optical and Magnetic Properties of Pure and Cerium Doped ZnO Nanoparticles by Sol Gel Method

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The Ce doped ZnO nanoparticles were used to study the structural, optical and magnetic properties. In this thesis, Pure and Ce doped Zinc oxide nanoparticles were prepared by sol-gel method. The as-formed ZnO nanoparticles (NPs) were characterized by Crystal structure (XRD), Surface morphology (SEM), Optical spectroscopy (UV-Vis) analysis and VSM studies. The wt% of cerium doping concentration increases while the average crystal sizes are increased upto 8 wt% and then crystal size increased in 10 wt% of doping level. The minimum average crystal size obtained from 8 wt% (8 nm). The absorption peak located at strong blue emission region and this region are energy level increased with decreased band gap in ZnO nanoparticles. SEM analysis shows that the Cerium doping generally spherical in shape with an average diameter of particle size. The enhanced intensity of the broad emission at green region confirms that the increased density of defects which can be attributed to the oxygen vacancy created by the existence of Ce impurities in ZnO nanoparticles. From VSM contemplates, Ce-doped ZnO NPs show clear room temperature ferromagnetic.

Essential Oil Blended Moringa Gum Composite Films For Food Packaging Application

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Moringa Gum was blend with two different essential oils (clove and cinnamon oil) to get a thin composite film by solution cast method. The morphology of the films was studied using scanning electron microscope. Physio-mechanical properties were analysed and compared with the pristine film. From the obtained results, it was found that the water solubility, thickness, transparency, mechanical strength, antibacterial activity of the prepared composite films showed better improvement when compared to the parent film. On exact comparison, clove oil – moringa gum composite film has given overall best result that was followed by cinnamon-moringa gum composite film and pure moringa gum film due to the interaction of their functional groups. Thus, the synthesised films will act as an ideal material for food packaging application.

Phytochemical-Induced Band Gap Narrowing and Morphological Analysis of TiO_2 NPs Synthesized via Gymnemasylvestre Leaf Extract

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The development of sustainable and eco-friendly methods for synthesizing semiconductor nanoparticles has gained significant traction due to the limitations of conventional chemical routes. *Gymnemasylvestre*, a medicinal woody climber renowned in Ayurveda as "Gurmar" (sugar destroyer), contains a rich profile of bioactive phytochemicals, including gymnemic acids, flavonoids, and phenolics . These constituents serve as potent reducing and stabilizing agents for nanoparticle fabrication. In this study, titanium dioxide (TiO_2) nanoparticles were synthesized via a green route using *G. sylvestre* leaf extract. The optical properties were characterized using UV–Visible spectroscopy, and functional group interactions were identified through Fourier Transform Infrared spectroscopy. The structural phases and crystallite size were determined via X-ray Diffraction, while surface morphology and particle distribution were analyzed using Scanning Electron Microscopy. UV-Vis analysis revealed a broad absorption band at 390 nm. Tauc plot analysis indicated an optical band gap of 3.07 eV, showing a red shift compared to bulk anatase (3.2 eV) due to quantum size effects and surface defects. FTIR confirmed the characteristic Ti–O–Ti stretching vibration at 437.84 cm^{-1}, along with peaks at 1641.42, 2169.92, and 3342.64 cm^{-1}, verifying successful phytochemical capping and stabilization. The XRD pattern exhibited sharp diffraction peaks corresponding to the anatase phase of TiO_2. The average crystallite size, calculated using the Debye Scherer equation, confirmed the nano crystalline nature of the synthesized material. SEM micrographs displayed predominantly spherical and semi-spherical nanoparticles. The images revealed some degree of agglomeration, typical of plant-mediated synthesis, with a relatively uniform distribution of particle sizes in the nanometer range. The results demonstrate that *G. sylvestre* extract effectively modifies the electronic and structural properties of TiO_2. The reduced band gap and surface functionalization enhance the potential of these nanoparticles for visible-light-driven photo catalysis, environmental remediation, and antibacterial applications.

Keywords: Gymnemasylvestre, TiO_2, Narrow Band Gap, Environmental Remediation

Spectroscopic Characterization and NLO Properties of 2-Cyclopenten-1-one

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2-Cyclopenten-1-one was investigated using Gas Chromatography–Mass Spectrometry (GC–MS), Fourier Transform Infrared (FT-IR) spectroscopy, and nonlinear optical (NLO) analysis to elucidate its structural, vibrational, and optical properties. The GC–MS analysis confirms the molecular identity and high purity of the compound through the observation of a prominent molecular ion peak, along with a well-resolved fragmentation pattern that is characteristic of a cyclic α,β-unsaturated ketone system. The observed fragment ions arise from the cleavage of the carbon–carbon bonds and rearrangements within the conjugated ring, thereby validating the proposed molecular structure.

Mushroom Stabilized Biogenic Spherical Ceria Nanoparticles Synthesis and Characterization

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Green synthesis is considered as an eco-friendly method of synthesis due simple, low cost and environmentally safe process. An eco-friendly method using Mushroom extract as a source of effective reducing agent was reported to prepare ceria nanoparticles (CeO_2 NPs). According to X-ray diffraction (XRD) and transmission electron microscope (TEM), the synthesized ceria NPs exhibited a cubic structure and spherical shape with the size range of 30 nm. The absorption band of Ce–O at ~565 cm^{-1} in fourier transform infrared (FTIR) spectra confirmed the formation of ceria NPs. Synthesized ceria nanoparticles showed antibacterial activity against pathogenic bacteria. Therefore, ceria NPs may be explored for the formulation of new alternative antibacterial and anticancer agents. It can be further utilized as an effective corrosion inhibitor for mild steel.

Keywords: Ceria nanoparticles, XRD, TEM and Antibacterial activity

Liquid Ammonic Diffused Chemical Synthesis of Cerium Oxide Nanoparticles and their Characterization

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To study the morphology features of Cerium oxide nanoparticles, Ammonia diffused Microwave Oven method is followed. About 0.01 Molar solution of Cerium Ammonium Nitrate was dissolved in distilled water and place in Microwave Oven and the reaction successfully carried out. The structure of Ceria nanoparticles was confirmed Ultra-Violet Spectrum, Fourier transform infrared spectrum, and SEM morphology. From this method, spherical ceria nanoparticles with an average of 40 nm was obtained according to XRD. Synthesized ceria nanoparticles showed better antibacterial activity against pathogenic bacteria. Therefore, Microwave Oven method is suitable technique to fabricate Ceria Nanopartiles for Biomedical applications.

Keywords: Microwave Oven, Chemical Synthesis, Characterization, Ceria nanoparticles.

Banana Peel Extract Stabilized Biogenic Irregular Ceria Nanoparticles and Evaluation of their Antibacterial Activity

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Banana is a nutrient rich fruit readily available in Tamil Nadu. It has been regularly consumed due its mineral content. In this work, Banana Peel extract was used as a reducing and stabilizing agent for the synthesis Ceria Nanoparticles. The synthesized Ceria nanoparticles were characterized to confirm the structure using various spectral techniques such as UV-Visible, FTIR and XRD techniques. An eco-friendly method using Banana Peel extract as a source of effective reducing agent was reported to prepare ceria nanoparticles (CeO_2 NPs). This method proved that it is suitable method for the synthesis of Ceria Nanoparticles for Biological applications.

Keywords: Green Synthesis, Ceria nanoparticles, XRD, TEM, Banana Peel, Antibacterial activity

Liquid Ammonia Stabilized Chemical Synthesis of Zirconia (ZrO_2) Nanoparticles and their Characterization

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In this work, ammonium hydroxide is used as a reducing as well as stabilizing agent for the synthesis of Zirconium oxide nanoparticles from Zirconyl oxychloride. The synthesized sample was dried and annealed at 500℃ for 4 hours. Then, powdered sample was characterized by UV-Visible, FTIR, XRD and SEM morphology study. The spectral techniques confirmed formation of ZrO_2 nanoparticles and SEM images confirmed the irregular morphology of the sample. Therefore, Zirconium oxide Nanoparticles can be synthesized using ammonium hydroxide for required morphology features and applications.

Keywords: Zirconuim oxide, Nanoparticles, Morphology, Ammonium Hydroxide

Efficient Red-Emitting $NaSrTiNbO_6:Eu^{3+}$ Double-Perovskite Phosphors with 98% Thermal Retention for White LED Applications

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The development of thermally stable red-emitting phosphors is crucial for next-generation white light-emitting diodes (WLEDs) with superior color quality. In this study, novel Eu^{3+}-doped $NaSrTiNbO_6$ double-perovskite phosphors with remarkably low thermal quenching behavior were synthesized for warm-white LED applications. A series of $NaSr_{1-x}TiNbO_6:xEu^{3+}$ phosphors was prepared via a conventional high-temperature solid-state reaction route. Structural analysis using X-ray diffraction with Rietveld refinement and Raman spectroscopy confirmed the formation of a single-phase cubic double-perovskite structure with $Pm\bar{3}m$ symmetry. Photoluminescence investigations revealed intense red emission originating mainly from the hypersensitive $^5D_0 \rightarrow {}^7F_2$ transition of Eu^{3+} ions under near-UV (396 nm) and blue light excitation, suggesting the substitution of Eu^{3+} ions at the Sr^{2+} A-site with reduced local symmetry. The local environment and optical characteristics of Eu^{3+} ions were further examined through Judd–Ofelt (J-O) analysis, emission asymmetry ratios, and decay lifetime measurements. The optimized $NaSr_{0.92}TiNbO_6:0.08Eu^{3+}$ phosphor demonstrated excellent thermal stability, retaining nearly 98% of its initial emission intensity at 440 K, with an activation energy of 0.193 eV. The observed thermal quenching behavior was interpreted using the configuration coordinate model. Additionally, the phosphors exhibited favorable correlated color temperature values, CIE chromaticity coordinates of (0.60, 0.39) close to the NTSC red standard (0.67, 0.33), and a high color purity of about 90%, highlighting their potential as efficient red-emitting components for advanced WLED devices.

Keywords: Eu^{3+}-doped phosphors; Double perovskite; Red emission; Thermal stability; White LED applications

Sequences and series of Real Number

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This project focuses on the analytical study of sequences and series of real numbers, which form the foundation of Real Analysis and mathematical convergence theory. The work explores the concepts of boundedness, monotonicity, limits, and various types of convergence such as pointwise and uniform convergence. Special attention is given to convergence tests, Cauchy sequences, and the completeness property of the real number system. The project also examines the behavior of infinite series, including absolute and conditional convergence, and the role of power series in representing real functions. Through rigorous proofs and illustrative examples, this study aims to deepen understanding of the structure and properties of real sequences and series, highlighting their significance in advanced analysis and applied mathematics.

Keywords: Real numbers, convergence, Cauchy sequence, series, limits

Ammonia Hydroxide Stabilized Chemical Synthesis of Copper Oxode Nanoparticles and their Characterization

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In this study, it is aimed to fabricate the Copper oxide nanoparticles (CuO NPs) using Ammonium hydroxide as reducing agent to study the formation and morphology of CuO nanoparticles. About 0.1 Molar Copper Chloride solution was taken Synthesized CuO NPs were structurally analyzed by UV-Visible, FTIR, XRD and SEM mtechniques and confirmed their formation and structures. Therefore, CuO NPs can be easily synthesized using Ammonium hydroxide for specified morphology and it can be used for the biomedical applications.

Keywords: Ceria nanoparticles, XRD, TEM and Antibacterial activity

A Survey on Nanotechnology and Plant Interceded Metal Nanoparticles and its Applications

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Nanotechnologies assume a significant job in research and this nanotechnology are grouped into different kinds of nanomaterials. During the latest decades, the green blend of metal nanoparticles has tremendous essentialness of both scholarly research and advancement. In tranquilize plant assume a significant job. The phytochemical present in the plant has productive in restoring and mending human infections. This customary technique is converged with metal. This blend of conventional and new technique defines green amalgamation. This strategy has high effect on social requirements for the relieving of human ills. The phytochemical present in the plant separate go about as topping and balancing out operator with metal to frame metal nanoparticles. Here, natural technique is conveyed which is superior to physical and compound strategy. This strategy is eco-accommodating, non-poisonous and simple to incorporate. Their application is stretched out in different fields and has distinctive topology.

Electronic and Structural Properties of Methyl 3-Hydroxyheptanoate: A UV–Vis and DOS Study

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Methyl 3-hydroxyheptanoate was investigated using UV–Visible spectroscopy**,** Density of States (DOS) analysis**, and** Density Functional Theory (DFT) based structural optimization to elucidate its electronic and molecular structural properties. The UV–Visible spectrum exhibits absorption bands in the ultraviolet region, which are attributed to $\mathbf{n} \rightarrow \boldsymbol{\pi}^*$ and $\boldsymbol{\pi} \rightarrow \boldsymbol{\pi}^*$ electronic transitions associated with the ester carbonyl group and the hydroxyl functionality. These transitions indicate the presence of localized and weakly delocalized electronic states within the molecule. The **DOS analysis** provides insight into the distribution of occupied and unoccupied electronic states, revealing clear separation between the valence and conduction regions. The dominance of oxygen-centered states near the frontier energy levels suggests their significant role in electronic transitions and chemical reactivity. The calculated energy gap reflects good molecular stability with moderate reactivity.

Selenization-Induced Lattice Reconfiguration and Electronic Transport Modulation in $Cu_2ZnGeSe_4$ Thin Films

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$Cu_2ZnGeSe_4$ (CZGSe), a quaternary chalcogenide semiconductor, has emerged as a promising photovoltaic material due to its earth-abundant constituents, tunable band gap, and superior optical absorption characteristics. In the present study, CZGSe thin films were deposited using a two-stage route involving electron-beam evaporation of stacked precursor layers followed by controlled in-situ selenization. The effect of selenization temperature on structural ordering, phase stability, microstructural evolution, and optoelectronic response was examined in detail.X-ray diffraction analysis revealed a well-defined tetragonal stannite phase, with optimal crystallinity achieved around 450 °C. Raman spectra corroborated phase purity and confirmed the suppression of secondary phases typically observed in kesterite derivatives. SEM imaging showed uniform, densely packed grains, while EDS and SIMS confirmed near-stoichiometric composition with a slight Cu-poor, Zn-rich profile—favorable for enhanced absorber behaviour. Optical investigations using UV–Vis–NIR spectroscopy yielded a direct band gap of ~1.6 eV, suitable for single-junction solar cells and photonic applications. Hall measurements revealed p-type conductivity with improved carrier mobility and reduced resistivity, indicating efficient charge transport pathways.The combined structural and functional analysis demonstrates that optimized thermal processing plays a crucial role in tailoring the defect chemistry, crystallographic stability, and optoelectronic performance of CZGSe films. These findings establish CZGSe as a viable material candidate for next-generation photovoltaic absorbers and advanced optoelectronic devices.

Keywords: CZGSe, thin films, selenization, optical properties, photovoltaic materials

Structural and Vibrational Properties of 3,4-Anhydro-D-galactosan: GC–MS, FT-IR and DFT Approach

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3,4-Anhydro-D-galactosan was investigated using Gas Chromatography–Mass Spectrometry (GC–MS) and Fourier Transform Infrared (FT-IR) spectroscopy, complemented by Density Functional Theory (DFT) calculations, to elucidate its molecular structure and vibrational characteristics. The GC–MS analysis confirms the molecular identity of the compound through the observation of a characteristic molecular ion peak and a well-defined fragmentation pattern, which is consistent with the anhydro sugar framework and supports the proposed molecular formula and purity.

Vertex cover problem of Cartesian product of networks

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Let G be a network, any node $v \in V(G) \backslash D$ is adjacent to atleast one node in D, then the set D is named a dominating set, represented by $\gamma(G)$. A set D of nodes in a network G is called an independent dominating set if D is an independent set. A total dominating set of a network G is a set D of nodes such that every nodes in G is adjacent to a node in D.A dominating set D of G is called paired dominating set whose induced graph of D contains a perfect matching. A 2-dominating set of a network G is a dominating set, in which any node not in D has minimum two neighbors in D. The minimal size of a 2-dominating set of G denoted by $\gamma_2(G)$, is the 2-domination number of G. The vertex cover problem is a fundamental concept in graph theory with applications in network security, biology, communication systems, and optimization. This paper studies the vertex cover properties of the Cartesian product of graphs, an important graph operation that combines two graphs to form a larger and more complex structure. We explore how the vertex cover number behaves under Cartesian products and identify relationships between the vertex cover numbers of the individual factor graphs and their product. Basic bounds, illustrative examples, and special cases such as grids, ladders, and hypercubes are discussed. The findings help in understanding how structural features of component graphs influence the vertex cover number of their Cartesian product, offering useful insights for theoretical research and practical problem-solving.

AMS subject classification:05C69,05C76,05C90.

Keywords: Domination; vertexcover; 2-domination; Cartesian product;

Investigation on inorganic potassium lithium sulfate single crystal grown by SR method and its characterization for nonlinear optical and photonic applications

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Inorganic crystal lithium potassium sulfate (LKS) was grown by Sangaranarayanan-Ramasamy technique. Structural parameters of the grown LKS crystal were confirmed by single crystal X-ray diffraction analysis. LKS crystal belongs to hexagonal system with non-centrosymmetric space group P63. The functional elements presented in the compound were analyzed by ICP-OES test. Thermal property of the sample was evaluated by tracing TGA and DSC plots. UV–Vis spectral studies revealed the lower cut-off wavelength, transparency and band gap (4.9 eV) of LKS crystal. Multi-shot laser damage threshold value of LKS crystal was found to be 4.2 GW/cm2. Using Kurtz and Perry powder technique, the second harmonic generation (SHG) efficiency was found. The photoluminescence, dielectric, mechanical and etching studies were also studied to test the LKS crystal for NLO application..

Keywords: Semi-organic material -spectral studies- thermal property

NMR and HOMO–LUMO Analysis of 2-Furanmethanol, 5 Ethenyltetrahydro α,α,5-Trimethyl-, trans

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2-Furanmethanol, 5-ethenyltetrahydro-α,α,5-trimethyl-, trans was analyzed using Nuclear Magnetic Resonance (NMR) spectroscopy and Density Functional Theory (DFT) based HOMO–LUMO analysis to elucidate its structural and electronic characteristics. The ^{1}H and ^{13}C NMR spectra display well-resolved signals corresponding to the furan ring protons, vinyl (ethenyl) group, hydroxymethyl moiety, and trimethyl-substituted tetrahydro framework, confirming the proposed molecular structure and trans configuration. Chemical shift values and splitting patterns reflect the influence of the heteroaromatic ring and alkyl substitution on the local electronic environment. DFT calculations were employed to optimize the molecular geometry and to evaluate the frontier molecular orbitals.

Spectroscopic and Frontier Orbital Analysis of 1,6-Octadien-3-ol, 3,7-dimethyl

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1,6-Octadien-3-ol, 3,7-dimethyl was investigated using spectroscopic techniques and Density Functional Theory (DFT) calculations to understand its structural and electronic properties. The FT-IR spectrum confirms the presence of hydroxyl and olefinic functional groups, while HOMO–LUMO analysis reveals charge distribution mainly over the unsaturated carbon chain. The calculated energy gap indicates good molecular stability with moderate reactivity, supporting its applicability in flavor, fragrance, and organic synthesis applications.

GC–MS, NBO Analysis and Mulliken Charge Distribution of trans-Limonene Oxide

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Gas Chromatography–Mass Spectrometry (GC–MS) and Density Functional Theory (DFT)-based electronic structure analyses were used to study trans-limonene oxide in order to determine its molecular identity and charge distribution properties. Through the presence of a distinctive molecular ion peak and a fragmentation pattern consistent with the epoxidized monoterpene framework, the GC–MS analysis verifies the compound's molecular composition and purity.Natural Bond Orbital (NBO) analysis was used to obtain a deeper understanding of the electronic structure. It revealed important intra-molecular charge transfer interactions between donor–acceptor orbitals, especially between the epoxide oxygen atoms and nearby carbon atoms. These interactions demonstrate electron delocalization within the system and aid in the stabilization of the molecular framework. The Mulliken charge distribution analysis indicates notable negative charge accumulation on the oxygen atoms, identifying them as potential reactive sites, while the carbon atoms of the terpene skeleton exhibit partial positive charge.

A Comprehensive Study on Determination of Total Hardness and Ions Present in Water in Kurinjipadi

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Water is an essential natural resource required for domestic, agricultural, and industrial purposes. The quality of groundwater is greatly influenced by the presence of dissolved salts and ions, which may affect its suitability for human consumption and irrigation. The present study aims to determine the total hardness and major ionic constituents of groundwater samples collected from Kurinjipadi and surrounding regions, including Vadalur, Serakuppam, Pacharapalayam, and Teerthanagiri. A total of five representative water samples were analyzed to evaluate their physicochemical characteristics and compliance with drinking water standards. The analysis included parameters such as total hardness, pH, electrical conductivity (EC), calcium, magnesium, chloride, fluoride, potassium, and sodium, and the observed values were compared with the permissible limits prescribed by the Bureau of Indian Standards (BIS). Total hardness was estimated using the EDTA titrimetric method employing Eriochrome Black-T as an indicator under controlled pH conditions. The results revealed that total hardness ranged from 56 mg/L to 300 mg/L, indicating variations from soft to moderately hard water. The pH values ranged from 7.0 to 7.7, confirming the slightly alkaline nature of groundwater samples. Electrical conductivity values varied between 177 µS/cm and 1072 µS/cm, indicating differences in dissolved ionic content. Notably, the fluoride concentration in Serakuppam (4.0 mg/L) exceeded the BIS permissible limit, posing potential health risks such as dental and skeletal fluorosis. Higher sodium and chloride concentrations observed in Pacharapalayam and Teerthanagiri suggest possible salinity intrusion and anthropogenic contamination.The study concludes that groundwater from Kurinjipadi and Vadalur is comparatively suitable for domestic use, whereas Serakuppam, Pacharapalayam, and Teerthanagiri require treatment and continuous monitoring to ensure safe utilization.Ke**ywords:** Groundwater Quality, Total Hardness, EDTA Titration, Calcium Ions, Magnesium Ions, Fluoride Contamination, Electrical Conductivity (EC), Physicochemical Parameters.

GC–MS, Mulliken Charge Distribution and Frontier Orbital Analysis of Bicyclo[2.2.1]heptan-2-ol, 1,5,5-trimethyl-

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Bicyclo[2.2.1]heptan-2-ol, 1,5,5-trimethyl- was investigated using Gas Chromatography–Mass Spectrometry (GC–MS) and Density Functional Theory (DFT) calculations to elucidate its structural and electronic properties. The GC–MS analysis confirms the molecular identity and purity of the compound through the observation of a characteristic molecular ion peak and a fragmentation pattern consistent with the bicyclic alcohol framework. Mulliken charge distribution analysis reveals significant charge localization on the oxygen atom of the hydroxyl group, indicating its role as a potential reactive site.

FT-IR and Molecular Docking Studies of trans-4-Methoxy Thujane against Liver Cancer-Related Receptors

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The compound trans-4-methoxy thujane (MMDT) was investigated using Fourier Transform Infrared (FT-IR) spectroscopy and molecular docking studies to evaluate its structural features and biological interaction potential. The FT-IR spectrum confirms the presence of characteristic functional groups, with prominent absorption bands corresponding to C–H stretching vibrations, C–O stretching of the methoxy group, and skeletal vibrations of the thujane framework, supporting the proposed molecular structure.the combined FT-IR and molecular docking investigations suggest that trans-4-methoxy thujane exhibits structural stability and promising interaction potential with liver cancer–related receptors, highlighting its possible relevance in drug discovery and medicinal chemistry applications.

FT-IR, Molecular Docking and Ramachandran Plot Analysis of Bicyclo[2.2.1] heptan-2-ol, 1-methyl-, acetate

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Fourier Transform Infrared (FT-IR) spectroscopy and in-silico molecular docking studies were used to examine the structural characteristics and potential biological interactions of bicyclo[2.2.1]heptan-2-ol, 1-methyl-, acetate. The presence of the acetate ester functionality within the bicyclic framework is confirmed by the FT-IR spectrum, which displays distinctive absorption bands corresponding to ester carbonyl (C=O) stretching, C–O vibrations, and aliphatic C–H stretching modes.To assess the compound's binding affinity toward particular biologically significant receptor proteins, molecular docking studies were conducted. Stable ligand-receptor complexes with favorable binding energy values are revealed by the docking results, suggesting efficient intermolecular interactions dominated by hydrophobic contacts and hydrogen bonding. Ramachandran plot analysis was used to further validate the structural reliability of the receptor models, demonstrating that the majority of amino acid residues fall within the most preferred.

FT-IR, UV–Visible and HOMO–LUMO Analysis of Isosorbide Dinitrate

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Isosorbidedinitrate was investigated using FT-IR and UV–Visible spectroscopy along with DFT-based HOMO–LUMO analysis to understand its vibrational and electronic properties. The FT-IR spectrum shows characteristic absorption bands corresponding to **nitrate ester (–ONO_2)** functional groups, confirming the molecular structure. UV–Visible spectral analysis reveals absorption bands in the ultraviolet region attributed to **n → π*** electronic transitions. HOMO–LUMO analysis indicates that the frontier orbitals are mainly localized over the nitrate moieties and isosorbide framework. The calculated **energy gap** suggests good molecular stability with moderate reactivity. The combined experimental and theoretical results provide valuable insight into the electronic behavior and stability of isosorbidedinitrate, supporting its pharmaceutical relevance.

Effect of Calcination Temperature on the Structural and Optical Properties of MnO_2 Nanoparticles

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Manganese (MnO_2) nanostructures of various sizes have been synthesized using sol–gel method followed by calcination of the samples from 500 to 800 °C. with the help of salt such as sulfates under a fine control of pH by using NaOH solution. The calcined MnO_2 powder samples were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FT-IR), UV–visible spectroscopy (UV–vis.) and thermogravimetric differential thermal analysis (TG-DTA). The average diameter of the MnO_2 nanostructures calcined at 500, 600, 700 and 800 °C was calculated to be 14-36 nm, respectively. Particle size and surface morphology of the synthesized manganese dioxide nanoparticles were analyzed using transmission electron microscope. The characteristic functional groups present in the molecule of synthesized nanoparticles were analyzed using Fourier Transform Infrared Spectroscopy. The optical property of the product has been explored by UV-Visible absorption and Thermogravimetric analysis has been performed to determine the thermal stability of the as-prepared MnO_2 samples.

Keywords: Pure MnO_2, XRD, TEM, FTIR, UV-vis, and TG-DTA.

Synthesis of Imidazole and Quinoxaline Enabled by Benzil

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A library of functionalized pyrrolidine-based NHC triazolium salts containing a BF_4 counterions have been prepared from readily accessible 2-pyrolidinone in one-pot reactions. Detailed mechanistic pathway was studied by isolating some stable imine-ether and hydrazone intermediates. Mechanistic investigation helps to improved synthetic protocol afforded increased yields for known NHC- triazolium structures and xx new NHCs were prepared using this protocol. The presence of a hydroxyl functional group on the NHCs has potential for further functionalization and for non-covalent control over catalytic reactions in which the NHCs can serve as organocatalyst or ligands for organometallic catalysis. For the important potential application of synthesized NHC organocatalyst have been examined in benzoin condensation, this catalytic system was studied by testing various solvents, catalyst and base loading effects to prepare broad range of functionalized benzoin compounds with high yields used by highly reactivetriazolium salts. EDG and EWG substituted α-hydroxy ketone derivatives were covered to corresponding benzil scaffolds under mild condition with MnO_2 as an oxidating reagent. Selective heterocycles, benzopyrazine and imidazole precursor were achieved from benzil compounds under mild conditions.

Ke words Catalysed, NHCs, Triazolium and Ambient reaction condition.

Pentapartitioned Neutrosophic Fuzzy Ideal of Near-Ring

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In this article, the concept of Pentapartitioned Neutrosophic Fuzzy Ideal of Near-Ring is introduced and examined few algebraic features such as union and intersection of Pentapartitioned Neutrosophic Fuzzy Ideal of Near-Ring. Additionally, we discuss about the homomorphic image and pre image of Pentapartitioned Neutrosophic Fuzzy Ideal of Near-Ring.

Keywords: Pentapartition, Neutrosophic Fuzzy Set, Pentapartitioned Neutrosophic Fuzzy Ideal of Near-Ring.

Electronic Structure and Charge Distribution Analysis of 1-Nitro-2-acetamido-1,2-dideoxy-D-mannitol Using DFT

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The structural, electronic, and spectroscopic properties of 1-nitro-2-acetamido-1,2-dideoxy-D-mannitol have been studied through theoretical and experimental methods. Key functional groups and vibrational modes connected to nitro, acetamido, and hydroxyl moieties were identified using Fourier Transform Infrared (FT-IR) spectroscopy. To support vibrational assignments and optimize the molecular geometry, Density Functional Theory (DFT) calculations were carried out. The electronic characteristics, such as the HOMO–LUMO energy gap and charge transfer behavior, were revealed by frontier molecular orbital analysis. The reactive sites and intramolecular charge delocalization within the molecule were identified by Mulliken charge distribution analysis. The combined experimental and theoretical findings demonstrate the impact of nitro and acetamido substituents on the electronic structure and validate the molecular stability. These results imply that this compound may be useful in pharmaceutical and biochemical applications.

Density Functional Theory and Spectroscopic Analysis of Ethanethioic Acid, S-(tetrahydro-2H-pyran-3-yl) Ester

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The structural, electronic, and spectroscopic properties of ethanethioic acid, S-(tetrahydro-2H-pyran-3-yl) ester, which was extracted from plant sources, were thoroughly examined using a combination of theoretical and experimental methods. Quantum chemical calculations and experimental FT-IR and UV-visible spectroscopy were used to optimize the molecular geometry, complete characterization of the fundamental vibrational modes, and detailed vibrational assignments. The B3LYP functional with the 6-311++G(d,p) basis set was used in Density Functional Theory (DFT) calculations to obtain the optimized geometry and theoretical vibrational wavenumbers, which demonstrated good agreement with experimental data.

Structural, Optical and Electrochemical behavior of Tin Oxide (SnO2) nanoparticles

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In this research work on structural, optical and electrochemical investigations of tin dioxide nanoparticles were synthesized by a chemical precipitation technique in different calcinations. The as synthesized SnO_2 nanoparticles were annealed at 700°C to 900°C for 2 hrs in ambient conditions. The crystallinity, grain size, surface morphology, optical and Capacitive behaviors of the samples were investigated by X-ray diffraction, scanning electron microscope, energy dispersive X-ray spectroscopy, transmission electron microscopy, UV-Visible diffuse reflectance spectroscopy, photoluminescence and cyclic voltammetry studies. It has been found that the different temperature played important role in controlling the crystallite size of SnO_2 nanoparticles. The XRD analysis showed well crystallized tetragonal structure SnO_2 nanoparticles. The broadband visible emission band is observed in the entire PL spectrum and the estimated energy band gap is about 3.52 eV. The origin of the luminescence is assigned to the recombination of electrons in a conduction band with holes in the $V_o^{\cdot\cdot}$ center. Experimental results reveal that increasing calcining temperature can decrease the oxygen vacancies related luminescence intensity of the sample. The specific capacitance (SC) is found to increase with an increase in different temperature. A maximum Specific capacitance value of 122 F/g is obtained scan rate for a 5 mV/s in SnO_2 composite at 700°C.

Keywords: SnO_2 nanoparticles, XRD, SEM, HR-TEM, UV-DRS, PL, CV.

FT-IR, FT-Raman and TD-DFT Studies on trans-2-Cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)- and 9,9-Dihydroxynonanoic Acid

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A thorough theoretical understanding of the molecular characteristics of trans-2-cyclohexen-1-ol, 2-methyl-5-(1-methylethenyl)-, and 9,9-dihydroxynonanoic acid was obtained through quantum chemical studies based on Density Functional Theory (DFT). The DFT method was used to optimize the molecular geometry, and important geometrical parameters were assessed. The fundamental vibrational modes were identified with the aid of Potential Energy Distribution (PED) analysis using VEDA software, and vibrational spectral analyses were carried out using experimental FT-IR and FT-Raman techniques. Using TD-DFT/B3LYP with the 6-311++G(d,p) basis set, electronic absorption spectra were calculated in the gas phase and different solvent environments (water, ethanol, ethyl ethanoate, acetone, and DMSO), and corresponding energy band gaps were assessed. The HOMO–LUMO energy gap, global hardness, softness, and electrophilicity index were estimated using Frontier Molecular Orbital (FMO) analysis.

Some studies in the theory of graphs

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Graph theory is an important branch of discrete mathematics with extensive application in computer science, engineering, and network analysis. This project presents a study of some selected topics in the theory of graphs. Focusing on fundamental concepts and structural properties. The study includes basic definition, types of graphs, degree of vertices, paths, cycles, connectivity, trees and graph Coloring. Important results and theorems are discussed with suitable illustration to provide better understanding. Application of graph theory in real- life situations such as communication networks and scheduling problems are also highlighted. The main objective of this project is to develop a strong theoretical foundation in graph theory and to demonstrate it's importance in solving practical problems.

Keywords: Graph theory, types of graphs, degree of a vertex, paths and cycles, connectivity, trees, Graph Coloring, chromatic number, applications of graphs.

A Study on Random Variables and Probability Distributions

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This project presents a study on random variables and probability distributions, which form an essential part of probability theory. Random variables are classified into discrete and continuous types, and their respective probability distribution functions are discussed. Important distributions such as the Binomial, Poisson, and Normal distributions are explained along with their fundamental properties. It also covers the computation of statistical measures including mean, variance, and moments.These measures help in analyzing and interpreting random phenomena. Applications of probability distributions in areas such as population studies, queueing systems, and statistical data analysis are briefly highlighted. This study aims to provide a clear understanding of probability distributions and their practical significance in mathematics and applied sciences.

Structure Theorem for Finite Abelian Groups

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The Structure Theorem for Finite Abelian Groups is a fundamental result in abstract algebra that describes the classification of finite abelian groups. This theorem states that every finite abelian group can be expressed as a direct sum of cyclic subgroups of prime power order. The project explains both the primary decomposition form and the invariant factor form of the theorem. It also discusses the uniqueness of these decompositions up to isomorphism. Several examples are provided to illustrate how to decompose a given finite abelian group. Applications of the theorem in number theory and linear algebra are briefly highlighted. This study helps in understanding the internal structure and classification of finite abelian groups in a systematic way.

A Study on some contribution to topology indices of graphs and related aspects

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Graph theory plays a significant role in modern mathematics and its applications, particularly in chemistry, computer science, and network analysis. Among various graph invariants, topological indices are numerical parameters that characterize the structural properties of graphs. These indices are widely used in chemical graph theory to study molecular structure-property relationships and quantitative structure-activity relationships (QSAR/QSPR).The present study focuses on some contributions to topological indices of graphs and their related aspects. It includes the investigation of degree-based, distance-based, and neighborhood-based topological indices such as the Zagreb indices, Randić index, Wiener index, Harary index, and other derived variants. New bounds, exact values, and mathematical properties of these indices are established for specific classes of graphs.Relationships between different indices and their structural implications are also examined.Further, the study explores applications of these indices in modeling chemical compounds, analyzing network structures, and solving combinatorial problems. The results contribute to a deeper understanding of graph invariants and open new directions for research in theoretical and applied graph theory.

Keywords: Topological indices, Graph invariants, Zagreb index, Randić index, Wiener index, Harary index, Degree-based indices, Distance-based indices, Chemical graph theory, QSAR/QSPR, Network analysis.

An Integrated CPM–PERT Based Decision Model for Time and Cost Optimization in District-Level Tourism Project Planning

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Choosing the best tourist destination requires careful planning of travel routes and efficient use of time. This project aims to identify the most appropriate tourist location among the key districts of Tamil Nadu by applying concepts from *graph theory* and *project management techniques*. In the proposed framework, each district is modeled as a node, and the connecting travel routes are represented as weighted edges based on distance or travel time. The Floyd–Warshall algorithm is employed to determine the shortest paths between every pair of districts. Additionally, the *Program* Evaluation and Review Technique(PERT) is used to manage scheduling activities and handle uncertainties in travel duration by identifying the critical path. The combined application of these methods provides a structured and *optimized approach to tourism planning*, enabling better decision-making and efficient itinerary design.

Keywords: Floyd-Warshall Algorithm, PERT, CPM, Graph Theory, Shortest Path Analysis, Tourism Optimization

A Study of Counting Principle in Algebraic Structures

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The counting principle is a fundamental concept in algebra and discrete mathematics used to determine the total number of possible outcomes in a multi-step process. It provides a simple algebraic method for counting without listing all possibilities. The principle is based on the idea of independent choices and their multiplication. This project explains the fundamental and generalized counting principles with mathematical justification. Various examples are included to demonstrate its practical use in algebraic problems. Applications in probability theory, computer science, and real-life situations are discussed. The project also highlights the connection between counting principles and permutations and combinations. Limitations of the principle are briefly examined. Special attention is given to avoiding over-counting. Overall, the project emphasizes the importance of the counting principle in mathematical problem solving.

Green Synthesis of Zno-Nanoparticles Using Catharanthus Roseus Leaf Extract and their Photocatalytic Degradation Activity

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The present study biosynthesized ZnO-NPs using *Catharanthus roseus* leaf extract at various concentration of 5, 10 and 15ml The synthesized ZnO-NPs are characterized by using UV-visible spectroscopy, XRD, HR-TEM, FT-IR and PL technique. ZnO-NPs as photocatalyst is used for the degradation of methylene blue dye. XRD results confirmed the effectiveness of the synthesis processes, demonstrating the production of single crystalline ZnO-NPs with hexagonal wurtzite structure. Morphology of ZnO-NPs revealed the spherical shape of the particles with different diameters. FT-IR spectra for *Catharanthus roseus* leaf extract clearly indicated the presence of bio-organic molecules such as, carboxylate group with proteins acted as a surfactant and stabilizes ZnO-NPs. The biosynthesized ZnO-NPs were effective photocatalyst for the degradation of methylene blue dye. Hence, it is clear that the biosynthesized ZnO-NPs along with *Catharanthus roseus* leaf extract is one of the best candidates for environmental application and various biological and medicinal related applications.

Random Events and Random Variables

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Probability deals with uncertainty in everyday life. A random event is an outcome of an experiment that cannot be predicted with certainty, such as tossing a coin or rolling a die. These events form the basis of probability theory. A random variable is a numerical value assigned to each possible outcome of a random experiment. It helps convert real-life random results into numbers for analysis. Random variables are mainly of two types: discrete and continuous. Discrete random variables take countable values, like the number of heads in coin tosses, while continuous random variables take values within a range, like height or time. By using random variables, we can calculate probabilities, averages, and variations, which are useful in science, engineering, economics, and daily decision-making. Thus, random events and random variables help us understand and manage uncertainty in a systematic way.

Keywords: Random Event, Probability, Random Experiment, Random Variable, Discrete Variable ,Continuous Variable, Outcome, Uncertainty.

Application of topology to data analysis

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Topological methods are revolutionizing data analysis by extracting insights from complex, high-dimensional datasets. Techniques like persistent homology and the mapper algorithm reveal patterns, clusters, and anomalies, offering a unique perspective on data shape and structure. These methods are applied across various domains, including image analysis, network science, and time series data, enabling researchers to identify meaningful features and relationships that traditional methods often miss. By focusing on the intrinsic topological properties of data, these approaches provide robust and interpretable results, even in noisy or incomplete datasets. This abstract highlight the power of topology in uncovering hidden structures and driving new discoveries in data-driven research.

Fermatean Fuzzy Filters In Sheffer Stroke Hilbert Algebras

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This study focuses on the development of Fermatean fuzzy structures within the framework of Sheffer stroke Hilbert algebras. Based on the theory of Fermatean fuzzy sets, the notions of Fermatean fuzzy filters and Fermatean fuzzy deductive systems are formulated and examined. Several algebraic properties associated with these concepts are derived and analysed. Criteria ensuring the formation of Fermatean fuzzy filters from Fermatean fuzzy sets are obtained, along with structural descriptions of such filters. Methods for generating Fermatean fuzzy filters using collections of classical filters are also presented. Moreover, the stability of Fermatean fuzzy filters under set-theoretic operations such as union and intersection is discussed. The effect of homomorphisms on Fermatean fuzzy filters is investigated, and the connection between Fermatean fuzzy filters and Fermatean fuzzy deductive systems in Sheffer stroke Hilbert algebras is established.

Keywords: Sheffer stroke Hilbert algebra,deductive system, filter, Fermatean fuzzy deductive systems, Fermateanfuzzy filter

Prediction of anti-Flaviviral drugs against zika virus using Degree-Based Topological indices in QSPR Modeling

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This research focuses on a set of potential therapeutic drugs active against the Zika virus, namely Mefloquine, Sertraline, Niclosamide, Tizoxanide, PHA-690509, Ribavirin, Emricasan, and Sofosbuvir. In this work, several degree-based topological indices were computed for these compounds, and quantitative structure–property relationship (QSPR) models were developed using line arregression techniques. These models were used to explore the relationship between molecular structure and twelve selected physicochemical properties. The analysis indicates that the Randic index $R(G)$ provides the most accurate predictions for boiling point, enthalpy of vaporization, flash point, and molar volume. The first Zagreb index $M_1(G)$ shows strong predictive performance for molar refractivity and polarizability, while the hyper-Zagreb index $H(G)$ effectively estimates surface tension. Furthermore, both the Sombor $S(G)$ and geometric–arithmetic $GA(G)$ indices exhibit consistent correlations across various physicochemical parameters, highlighting their broad applicability in molecular property prediction.

Keywords: Topological indices; QSPR analysis; anti-flaviviral drugs.

A Study of Green's Function in Partial Differential Equation

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The objective of this project is to explain the concept of Green's function and their importance in solving linear partial differential equations. This study aims to derive Green's function using the Dirac delta function and to find Green's function for Laplace and Helmholtz equations under Dirichlet and Neumann boundary conditions. It also seeks to prove the existence, uniqueness and basic properties of solutions obtained using Green's function. Further, the project aims to explain and apply methods such as the method of images and eigen function expansions for constructing Green's function in standard domains. Finally, it aims to demonstrate and verify the theorems of Green's function in solving the problems.

Z-Scan Investigation of Growth and Optical Nonlinearities in Semi-Organic Strontium Diformate Single Crystal for Third-Order NLO Applications

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A semi-organic nonlinear optical (NLO) crystal of Strontium diformate (SDF) was successfully synthesized by reacting strontium chloride hexahydrate with sodium formate. Bulk crystals were grown using the solution growth technique. Structural analysis through single-crystal X-ray diffraction revealed that SDF crystallizes in the orthorhombic system with the space group P212121. Optical characterization was carried out using UV–Vis–NIR spectroscopy, while the crystal's thermal behavior, including stability and decomposition, was examined through TGA and DTA studies. The third-order nonlinear optical response of the crystal was investigated using the Z-scan method with a He–Ne laser operating at 632.8 nm. The measured third-order nonlinear susceptibility was 1.438×10^{-5} esu, and both the nonlinear refractive index and absorption coefficient were determined to assess its potential in optical limiting applications. Furthermore, the Kurtz powder test confirmed the presence of second harmonic generation (SHG) in the grown crystal.

Annona Squamosa Stabilized Synthesis of Silver Nanoparticles for Antibacterial Application

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Silver nanoparticles are used as antibacterial activity against many bathogenic bacteria and fungus. It also used for various biomedical applications. An eco-friendly method using *Annona squamosa* extract as a source of effective reducing agent was reported to prepare Silver Nanoparticles (AgNPs). The X-ray diffraction (XRD) showed spherical morphology with some irregular shapes. The transmission electron microscope (TEM) showed various fascinating shape. The UV-Visible spectrum showed maximum absorption at 420 nm further confirmed the formation of silver nanoparticles. It showed effective zone of inhibition against pathogenic bacteria at the concentration of 100 µg/ml. Therefore, Silver nanoparticles can be explored for the formulation of antibacterial agent.

Keywords: Silver nanoparticles, *Annona squamosa* XRD and Morphology

A study on fixed point theorems in different spaces and its applications

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Fixed point theory is an important branch of mathematical analysis with wide applications in various fields such as differential equations, optimization, game theory and economics. This study focuses on fixed point theorem in different mathematical spaces, including metric spaces, normal linear spaces, Banach spaces, and complete metric spaces. Fundamental results such as Banach 's Contraction Principle, Brouwer's Fixed Point Theorem, Schauder Fixed Point Theorem, and Kakutani'sFixed Point Theorem are discussed and analyzed. The application of these theorems in solving nonlinear equations, integral equations, boundary value problems and economic equilibrium models are presented. This study demonstrates how fixedpoint theory provides powerful tools for solving real-world mathematical problems across various disciplines.

Keywords: Fixed point theorem-Metric Space- Banach Space-Contraction mapping-Complete Metric Space-Brouwer Theorem-Schauder Theorem-Kakutani Theorem-Nonlinear Equations-Integral Equations-Economic Equilibrium.

Synthesis of Silver Nanoparticles using Tomato Extract as Stabilizing Agent and their Characterization

S.Rekha[a], R. Kavitha[a]*
[a, a*] *Department of Chemistry, Valliammai Women's College, Arakandanallur-605752*

Silver nanoparticles had drawn the attention of researcher due to its biological activity. An eco-friendly method using *Tomato* extract as a source of effective reducing agent was reported to prepare Silver nanoparticles (Ag NPs). Biosynthesized AgNPs were characterized by UV-Visible, FTIR, XRD and TEM techniques. The stretching frequency of Ag NPs and absorption maximum were confirmed by FTIR and UV-Visible spectra. TEM morphology study showed various shapes of nanoparticles, and hence it can be used as biomaterials for the development of antibacterial agent.

Keywords: Silver nanoparticles, Tomato extract, Morphology study, Characterization activity

Sustainable Synthesis of Silver-Doped Nano-Hydroxyapatite from Bio-Waste Derived Calcium Sources for Biomedical Applications

T U Jeevitha[a]

[a]*Department of Physics, AMET University, Chennai, India*

Hydroxyapatite (HAp) is a bioceramic material extensively used in orthopedic and dental applications due to its excellent biocompatibility, bioactivity, and structural similarity to natural bone mineral. In this study, a sustainable and eco-friendly route is proposed for the synthesis of silver-doped nano-hydroxyapatite (Ag-nHAp) using bio-waste–derived calcium sources as an alternative to conventional synthetic precursors. The valorization of biological waste materials as calcium resources not only reduces environmental burden but also promotes circular economy principles in advanced biomaterial development. The nano-hydroxyapatite was synthesized through a controlled wet chemical precipitation method, followed by silver ion incorporation to impart antimicrobial functionality. Structural and phase analysis confirmed the formation of crystalline hydroxyapatite with successful silver doping. Morphological studies revealed nanoscale particle formation with uniform distribution. The presence of silver enhances antibacterial performance against common pathogenic microorganisms while maintaining the inherent biocompatibility of hydroxyapatite. The developed Ag-nHAp demonstrates significant potential for applications in bone tissue engineering, implant coatings, dental restorations, and antimicrobial biomedical devices. This work highlights a sustainable strategy for transforming bio-waste into high-value functional nanomaterials, aligning green chemistry principles with biomedical innovation.

Keywords: Seashell, Nano hydroxyapatite, Silver doping, Green synthesis, Biomedical materials, Circular economy.

Pomegranate Peel Stabilized Biosynthesis of Silver Nanoparticles for Antibacterial Application

R.Monika[a], R. Kavitha[a]*

[a, a*] *Department of Chemistry, Valliammai Women's College, Arakandanallur-605752*

Silver nanoparticles are used as antibacterial activity against many bathogenic bacteria and fungus. It also used for various biomedical applications. An eco-friendly method using *Pomegranate Peel* extract as a source of effective reducing agent was reported to prepare Silver Nanoparticles (AgNPs). The X-ray diffraction (XRD) showed spherical morphology with some irregular shapes. The transmission electron microscope (TEM) showed various fascinating shape. The UV-Visible spectrum showed maximum absorption at 420 nm further confirmed the formation of silver nanoparticles. It showed effective zone of inhibition against pathogenic bacteria at the concentration of 100 µg/ml. Therefore, Silver nanoparticles can be explored for the formulation of antibacterial agent.

Keywords: Ceria nanoparticles, XRD, TEM and Antibacterial activity

A Comparative Study of Hardness of Water in Cuddalore District

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Water quality is a major determinant of public health and environmental sustainability, especially in regions dependent on groundwater sources. The present study aims to evaluate and compare the hardness and overall physicochemical characteristics of groundwater samples collected from selected areas of Cuddalore district, Tamil Nadu. Twenty water samples were collected from two major study regions, namely Kurinjipadi and surrounding areas (Kurinjipadi, Vadalur, Serakuppam, Pacharapalayam, and Teerthanagiri) and Neyveli and surrounding areas (Indra Nagar, Therkumelur, Abathanapuram, Marungur, and Thopoulikuppam). The analysis was carried out by employing standard analytical methods, including EDTA titrimetric technique for determining total hardness, calcium hardness, and magnesium hardness. Additional parameters such as pH, electrical conductivity (EC), chloride, fluoride, sodium, potassium, and total dissolved solids were also assessed to understand the suitability of groundwater for domestic and drinking purposes. The results indicate that groundwater quality varies significantly among the sampling locations. Comparative evaluation revealed that Neyveli and its surrounding regions exhibited higher mean total hardness, EC, calcium, chloride, sodium, and magnesium concentrations compared to Kurinjipadi regions, indicating greater mineralization and salinity. Risk scoring based on guideline exceedance identified Therkumelur and Teerthanagiri as high concern areas requiring immediate monitoring and remedial measures. Overall, the study highlights the need for regular groundwater quality assessment and implementation of suitable treatment techniques such as softening and defluoridation in vulnerable regions.

Ke**ywords:** Groundwater Quality; Water Hardness; EDTA Titration; Physicochemical Parameters; Total Dissolved Solids (TDS); Electrical Conductivity (EC); Fluoride Contamination.

Synthesis, Structural Characterization of Cobalt Doped Cerium Oxide Nanoparticles and their Characterization

R.Dhivyadharshini[a], R. Kavitha[a]*

[a, a] Department of Chemistry, Valliammai Women's College, Arakandanallur-605752*

In the present work, a facile synthesis of Cobalt dopped cerium oxide nanoparticles, characterization and optical property were explained. The synthesized nanoparticles were characterized using X-ray diffraction techniques (XRD), Ultra-violet spectrophotometer (UV-Vis), and Fourier transform infrared spectrophotometer (FTIR). The XRD reveals the crystalline nature of the nanoparticles with an average size of 10 nm. The Tem images showed spherical shaped nanoparticles. The FTIR result confirms the chemical bonding of Ce metal stretching with oxygen. From the result of these study, Co doped CeO_2 nanoparticles could be used a suitable nanomaterials for biological applications.

***Keywords**:* Cobalt, Ceria nanoparticles, Characterization, and Morphology

Ferromagnetic behaviour of Cobalt oxide (Co_3O_4) nanoparticles

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[a]Assistant Professor, IFET college of Engineering, Villupuram

Cobalt oxide (Co_3O_4) nanoparticles were synthesized via a co-precipitation method, and the influence of calcination temperature on their structural, morphological, optical, magnetic, and electrochemical properties was systematically investigated. X-ray diffraction analysis confirmed the formation of single-phase cubic Co_3O_4 nanoparticles, with crystallite size increasing at higher calcination temperatures. FTIR spectra revealed characteristic metal–oxygen vibrational modes below 1000 cm^{-1}, confirming the formation of cobalt oxide. FESEM images showed a morphological transformation from spherical to hexagonal-like structures with increasing calcination temperature, while EDAX mapping verified the presence of Co and O elements. Optical studies indicated two absorption bands corresponding to electronic transitions, with the optical bandgap decreasing as calcination temperature increased. BET analysis showed a high specific surface area of 155.88 m^2/g. Magnetic studies using VSM revealed weak ferromagnetic behaviour at lower temperatures, which improved with increased crystallite size. These results demonstrate that calcination temperature plays a crucial role in tuning the multifunctional properties of Co_3O_4 nanoparticles.

Catalytic Activity and Molecular Simulation Studies Toward the Development of Synthetic Routes for TrimericTriaryl Pyridinium Ionic Liquids

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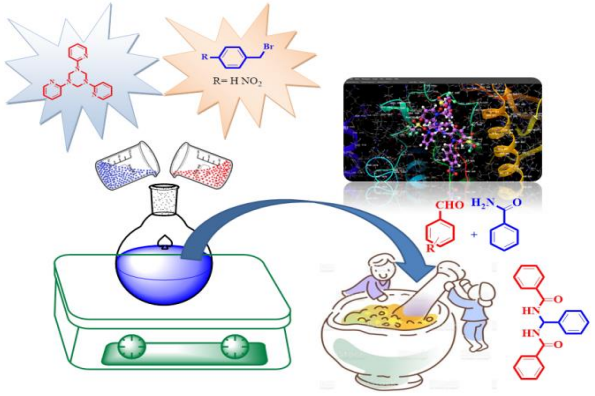
Water soluble trimeric pyridinium cation synthesis with various inorganic counter anions using conventional and silica supported Muffle furnace methods. The solvent-free synthesis approach improves the conventional method in terms of non-toxicity, quicker reaction time, ease of workup without purification, and greater yields. Synthesized trimeric substituted pyridinium salts are acted as excellent catalytic response for the preparation of Gem-bisamides derivative under conventional approach. To evaluate the molecular docking analysis of compounds 2a, 2b, 2c and 3b, 3c, 3d is possess the most potent VEGFR-2 kinase protein inhibitory activities, interestingly the compound **3b** strongly binding and regulate the VEGFR-2 kinase activity in therapeutic strategies and cancer prevention**.**

Keywords: Conventional, solid phase, anion exchange, molecular simulation, Gem-bisamides.



Fabrication of Pectin/Poly(vinyl alcohol)/Graphene oxide nanocomposite for effective removal of Methylene blue dye from aqueous solution: Kinetics and Isotherm study

V. Shanmuga Priya [a], S. Khaleel Basha [b], V. Sugantha Kumari [a*]
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We report a facile design and synthesis of Graphene oxide (GO) incorporated pectin/PVA nanocomposite (PPGO) by employing solution casting method.The fabricated nanocomposite was investigated by FT-IR, XRD, Raman, TEM, SEM and TGA-DSC. The potential of the prepared nanocomposite for effective removal of methylene blue dye from aqueous solution was investigated by performing a series of batch adsorption experiments to study the effect of adsorbent dosage, initial dye concentration, contact time and pH. The adsorption was influenced by the pH of the medium, indicating an electrostatic interaction between the adsorbent and MB molecules. The kinetics of adsorption followed a pseudo-second order model. The equilibrium adsorption capacity was found out to be 162 mg L^{-1}described by the Langmuir adsorption model. To evaluate the reuse of PPGO, desorption was performed. Due to its good adsorption efficiency, PPGO may be a promising adsorbent for removal of dye. **Keywords**: Graphene oxide, nanocomposite, adsorption, methylene blue.

Performance Evaluation of Cashew Nutshell Ash Aiming Their Use in Cement Composites

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[b]Department of Chemistry, School of Basic sciences, (VISTAS), Pallavaram, Chennai – 17
[c]Department of Civil Engineering, School of Engineering, (VISTAS), Pallavaram, Chennai – 17

Every year, the agro-industrial sector generates a lot of waste by-products that, due to poor management and a lack of awareness of their values, present risks to the environment, society,and economy. One of the promising substitute materials for cement that can be used in the construction industry is cashew nut shell waste. Thus, the ash from cashew nutshell was investigated in this work. Since they are a byproduct of the energy generation process, ashes maintain a significant position among the agro-industrial wastes. Because most ashes include pozzolanic activity, they can be utilized in place of cement to create low-cost composites withless energy waste. The current study uses Thermogravimetric analysis (TGA), and differential thermogravimetric analysis (DTGA), X-Ray Fluorescence Analysis (XRF) and X-Ray diffraction (XRD). It is concluded that using CNSAin concrete is beneficial in reducing environmental and sustainability issues. CNSA concrete is advantageous in environments with high sulfate concentration. It was found that the total amount of silicon oxide (SiO_2), aluminum oxide (Al_2O_3), and iron oxide (Fe_2O_3) obtained in CNSA. An amorphous structure is indicated by the broadened peak that occurs in the XRD pattern at about $2\theta=24^\circ$. Increasing the activation temperature tends to cause the activated carbon to graphitize. Chemical testing revealed a low silicon (SiO2) content, and the analysis of the CNSA-soluble extract revealed the presence of heavy metals.

Keywords: Cashew nut ashes; Agroindustrial waste; X-Ray diffraction; X-Ray Fluorescence Analysis; Thermogravimetric analysis

Comparative Study on Green Synthesis, Characterization, and Biological Applications of Cerium Oxide Nanoparticles Using Artabotrys hexapetalus, Justicia adhatoda, Gloriosa superba, and Murraya koenigii Leaf Extracts.

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Cerium oxide nanoparticles (CeO_2 NPs) have garnered significant attention due to their unique physicochemical properties, including high redox activity, oxygen storage capacity, and biocompatibility. Green synthesis methods utilizing plant leaf extracts offer an eco-friendly, cost-effective alternative to traditional chemical approaches, minimizing toxic byproducts and enhancing nanoparticle stability through natural capping agents. This review article compares the green synthesis, characterization, and biological applications of CeO_2 NPs derived from four medicinal plant leaf extracts: Artabotrys hexapetalus, Justicia adhatoda, Gloriosa superba, and Murraya koenigii. Drawing from recent studies, we highlight variations in synthesis protocols, nanoparticle properties (e.g., size, shape, and band gap), and applications such as antibacterial, anticancer, and photocatalytic activities. Comparative analysis reveals plant-specific influences on NP morphology and efficacy, underscoring the potential for tailored biomedical and environmental uses.

Keywords: Green Synthesis, Nanoparticles, Metal oxide, Biological Application

Nanomaterials at the Frontier of Corrosion Inhibition

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Corrosion is a major cause of material degradation, leading to economic loss and safety concerns in industrial systems.Traditional corrosion inhibitors and coatings often suffer from limited durability and environmental toxicity.Nanomaterials have emerged as advanced alternatives due to their unique structural and surface properties. Their high surface area enhances interaction with metal substrates and corrosive environments.Metal and metal oxide nanoparticles provide effective passivation and barrier protection.Carbon-based nanomaterials such as graphene and carbon nanotubes improve coating impermeability.Nanocomposites combine polymers and nanoparticles to achieve synergistic corrosion resistance..Green-synthesized nanomaterials address environmental and sustainability concerns. Bio-inspired nanomaterials show promise for eco-friendly corrosion inhibition.Smart nanomaterials respond to pH, redox, or mechanical stimuli. Such responsiveness enhances long-term corrosion protection efficiency. Nanomaterial-based coatings perform well in aggressive environments. They are effective in marine, chemical, and energy applications. Challenges include large-scale production and cost optimization. Long-term stability and compatibility with substrates require further study. Standardized testing methods are essential for industrial adoption. Overall, nanomaterials represent a frontier in advanced corrosion inhibition technologies.

Keywords: Nanomaterials; Corrosion inhibition; Nanocoatings; Nanocomposites; Self-healing materials; Green corrosion inhibitors

Synthesis, Characterisation Crystal XRD and DFT study of Ester derivative of Benzilic acid

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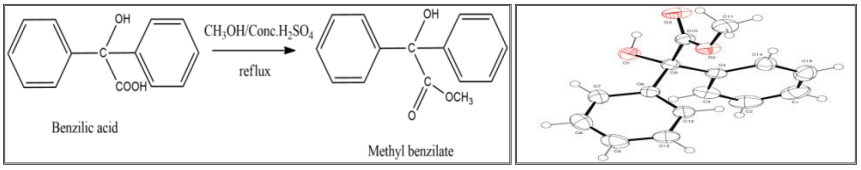
Ester derivative of Benzilicacid wassynthesised by esterification of benzilic acid on methanol.Methyl benzilate called as ster of benzylic acid, an important α-hydroxy ester with relevance in pharmaceutical and fine chemical synthesis, was successfully synthesized via esterification of benzilic acid under controlled reaction conditions. The synthesized compound was purified and characterized using Fourier-transform infrared spectroscopy (FT-IR), nuclear magnetic resonance (^1H and ^13C NMR) spectroscopy, and mass spectrometry, confirming its molecular structure and functional groups. Single-crystal X-ray diffraction (SC-XRD) analysis revealed that methyl benzilate crystallizes in a monoclinic crystal system, providing detailed insight into its molecular geometry, intermolecular interactions, and hydrogen-bonding network within the crystal lattice. Density Functional Theory (DFT) calculations were performed using the B3LYP functional with an appropriate basis set to optimize the molecular geometry and evaluate electronic properties. The theoretically optimized structure showed good agreement with the experimentally determined crystallographic parameters. Frontier molecular orbital (HOMO–LUMO) analysis indicated the electronic stability and reactivity of the molecule, while molecular electrostatic potential (MEP) mapping identified regions susceptible to electrophilic and nucleophilic attack. The combined experimental and theoretical investigations provide a comprehensive understanding of the structural, electronic, and crystallographic features of methyl benzilate, highlighting its stability and potential applicability in molecular design and synthetic chemistry.

Keywords: Ester derivative of Benilic acid, Characterisation, Crystal XRD and DFT



Analysis on Soret and MHD parabolic flow past an accelerated vertical plate without heat and mass diffusion in the presence of rotation

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Soret impact of rotational action on the unsteady MHD parabolic flow across an accelerating vertical plate with constant mass diffusion and uniform temperature. The fluid under consideration conducts electricity. The solutions for the profiles of velocity, temperature, and concentration have been found using the Laplace transform method. Various graphs for parameters such as the thermal Grashof number, the mass Grashof number, the Prandtl number, the Hartmann number, the Schmidt number, the Soret number, the time of magnetic field, and the acceleration parameter are used to describe the findings obtained. The velocity is expected to expand as the mass Grashof or heated Grashof number is estimated to grow. It is also verified that the velocity increases as the magnetic field strength decreases.

Keywords: Soret effect, vertical plate, parabolic, magnetic field, mass diffusion, Rotation

Super capacitor& Energy Storage of Co_3O_4 nanoparticles

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[a]Assistant Professor, IFET college of Engineering, Villupuram

Co_3O_4 nanoparticles were prepared using a facile co-precipitation technique, and the effect of calcination temperature on their electrochemical performance was evaluated for supercapacitor applications. Structural analysis by XRD confirmed the formation of cubic-phase Co_3O_4 nanoparticles, while FTIR spectra showed characteristic metal–oxygen vibrations. Morphological studies using FESEM revealed a transition from spherical to hexagonal-like structures with increasing calcination temperature, accompanied by an increase in crystallite size. EDAX mapping confirmed the elemental composition of cobalt and oxygen. Optical studies showed a reduction in bandgap energy with increasing calcination temperature, indicating enhanced electronic conductivity. BET analysis revealed a high surface area of 155.88 m^2/g, beneficial for charge storage. Electrochemical measurements demonstrated a high specific capacitance of 535 F g^{-1} at a scan rate of 5 mV s^{-1}, indicating excellent charge storage capability. The results suggest that Co_3O_4 nanoparticles synthesized via this method are promising electrode materials for high-performance supercapacitor applications.

A Study on Various Application in Differential Equation

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[a,a,]Department of Mathematics, Valliyammai Womens College of Arts and Science, Arankandanallur*

Many problems in engineering and science can be formulated in terms of differential equations.The formulation of mathematical models is basically to address real-world problems which has been one of most important aspects of appliedmathematics.To study some real-world problems which are described by first order differential equation.To apply logistic growth model of population which is expressed by first order nonlinear differential equation for population growth of animals when overcrowding and competition resources are taken into consideration.To discuss the use of mathematical model for harvesting renewable natural resource.To analyse and interpret some real-world application problems of first order linear and non-linear differential equations.

வள்ளியம்மை மகளிர் கலை மற்றும் அறிவியல் கல்லூரி

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முதுகலைப்படிப்பில் சேரும் அனைத்து மாணவிகளுக்கும், முதல் பருவக்கட்டணத்தில் 50% கட்டண சலுகை வழங்கப்படும்.

- குறைந்த கட்டணம்
- சிறந்த கல்வி
- கேன்டீன் வசதி உண்டு
- பேருந்து வசதி உண்டு

மாணவிகளுக்குச் சிறப்பு கட்டணச்சலுகை முதல் பருவம் மட்டும்

400 - 450 மதிப்பெண் பெற்ற மாணவிகளுக்கு 25%,
451 - 500 மதிப்பெண் பெற்ற மாணவிகளுக்கு 50%,
501 - மதிப்பெண்ணிற்கு மேல் பெற்ற மாணவிகளுக்கு 100%

மாணவிகளுக்கு புதுமைப்பெண் திட்டத்தின் மூலம் மாதம் ரூ.1000/- பெற்று தரப்படுகிறது.
மேலும் மாணவிகளுக்கு SC/ST, National Scholarship பெற்று தரப்படும்

2026 - 27ஆம் ஆண்டிற்கான சேர்க்கை நடைபெறுகிறது.
விண்ணப்பம் கல்லூரி அலுவலகத்தில் வழங்கப்படுகிறது.

ACADEMIC ACHIEVEMENTS OF STUDENTS

பல்கலைக்கழக தரவரிசையில் இடம் பெற்றோர் (University Rank Holders)

'தொட்டுப்பார் நான் காகிதம், படித்துப்பார் நான் ஆயுதம்'

என்பதற்கிணங்க முயற்சி என்ற சொல்லுக்கே முன்னுதாரணமாக நின்று, காகிதத்தில் தன் கைவண்ணத்தைக் காட்டி பல்கலைக்கழகத் தேர்வில் பதக்கம் வென்ற மாணவிகள்

P.SASIREKHA
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2014-2017 BATCH
IX RANK

K.LAKSHMI
B.A., TAMIL
2015-2018 BATCH
VI RANK

R.KANMANI
B.A.,TAMIL
2018 - 2019 BATCH
III RANK

E.BABY PRIYA
B.Com (G)
2018 - 2019 BATCH
IX Rank

S.NIVETHA
B.Sc.,Physics
2018-2021 BATCH
IV RANK

S.ABIRAMI
B.Sc., CHEMISTRY
2018-2021 BATCH
III RANK

S.NIVETHA
B.A.,TAMIL
2019-2022 BATCH
VI - RANK

K.A.BAKKIYALAKSHMI
M.A.,TAMIL
2019-2021 BATCH
VIII RANK

R.KANMANI
M.A.,TAMIL
2019-2021 BATCH
I RANK

K.AKILA
M.A., TAMIL
2019-2021 BATCH
III RANK

P.SASIREKHA
M.A.,TAMIL
2019-2021 BATCH
IV RANK

S.MANVIZHI
M.A., TAMIL
2020-2022 BATCH
X RANK

எம் கல்லூரியில் தமிழ்துறையில் படித்த கண்மணி என்னும் மாணவி இளங்கலை மற்றும் முதுகலை ஆகிய இரண்டு நிலைகளிலும் பல்கலைக்கழக தேர்வில் தங்கப்பதக்கம் வென்றுள்ளார்.

எங்கள் கல்லூரி மாணவிகள் முதல் முயற்சியிலேயே நுழைவுத் தேர்வில் தேர்ச்சி பெற்று Ph.D., மற்றும் CA (Chartered Accountant) படித்து வருபவர்கள்

R.Kanmani from Department of Tamil doing Ph.D,
N.Racshitha from Department of Mathematics completed Ph.D,
J.Ureshya from Department of Physics doing Ph.D,
M.Jayapriya from Department of Chemistry doing Ph.D,
M. Archana from Department of Commerce pursuing (CA)

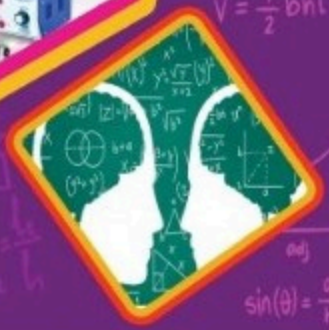
UNIVERSITY PLAYERS IN SPORTS

"உடல்நலமே உண்மையான செல்வம் - (Health is Wealth)"

"உடலினை உறுதி செய்" என்னும் மகாகவி பாரதியாரின் பொன்மொழிக்கேற்ப உடலினை உறுதி செய்யும் விளையாட்டுக்கு இக்கல்லூரில் முன்னுரிமை வழங்கப்படுகிறது. அவ்வகையில் எம் கல்லூரி மாணவிகள் விளையாட்டில் பல்கலைக்கழக அளவில் பங்கு கொண்டு பல வெற்றிகளை பெற்றனர். இதன்மூலம் அரசு பணியில் முன்னுரிமை பெற்று அரசு பணியில் உள்ளனர்.

வ. எண்.	விளையாட்டின் பெயர்	பல்கலைக்கழகத்தின் FORM - III சான்று பெற்ற மாணவிகள்	சான்று பெற்ற ஆண்டு
1	CRICKET	2	2015 - 16
2	BALL BADMINTON	1	2015 - 16
3	CRICKET	2	2016 - 17
4	HANDBALL	1	2016 - 17
5	BALL BADMINTON	1	2016 - 17
6	HAND BALL	1	2016 - 17
7	KHO-KHO	1	2016 - 17
8	CRICKET	3	2017 - 18
9	HANDBALL	1	2017 - 18
10	HOCKEY	1	2017 - 18
11	HAND BALL	1	2018 - 19
12	FOOTBALL	1	2018 - 19
13	TABLE TENNIS	1	2018 - 19
14	CRICKET	6	2018 - 19
15	HAND BALL	2	2019 - 20
16	CRICKET	6	2019 - 20
17	HOCKEY	1	2019 - 20
18	BALL BADMINTON	1	2019 - 20
19	FOOT BALL	2	2022 - 23
20	CRICKET	9	2022 - 23
21	BASKET BALL	2	2022 - 23
22	HAND BALL	2	2022 - 23
23	NETBALL	1	2022 - 23
24	CHESS	1	2022 - 23
25	BADMINTON	1	2024 - 25
26	BADMINTON	1	2024 - 25
	TOTAL	**52**	

இக்கல்லூரியில் Badminton மற்றும் Table Tennis-க்கு உள்விளையாட்டரங்கம் (Indoor Stadium) உள்ளது.



VALLIAMMAI WOMEN'S COLLGE OF ARTS AND SCIENCE

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