Proceedings of the International Conference on Spectroscopy, Materials & Observational Sciences

(ICOSMOS – 2025)

20th February, 2025

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Organised by

PG Department of Physics
DWARAKA DOSS GOVERDHAN DOSS VAISHNAV COLLEGE (SHIFT-II) (AUTONOMOUS)
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Arumbakkam, Chennai – 600106

In association with

Indian SpectroPhysics Association (ISPA), Chennai, India

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Founder President, ISPA

Dr. B. Sylaja, Ph.D.
Head i/c, Associate Professor, PG Department of Physics
DDGD Vaishnav College
Convenor, ICOSMOS - 2025

CREDITS

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About the Institution

Dwaraka Doss Goverdhan Doss Vaishnav College, a linguistic minority institution was established in the year 1964 for the cause of higher education. This institution has been a temple of learning for generations of enthusiastic learners through six decades and more. The curriculum has been updated periodically, concerned with the current trends in the diverse disciplines of arts, commerce, science and technology. It has been reaccredited with A++ Grade by NAAC.

About the Department

The Post Graduate Department of Physics is dedicated to excellence in teaching and is committed to serve the student community. The Department offers a degree in Bachelor of Science in Physics with Computer Applications (B.Sc PCA) since 2011 and Master of Science in Physics since 2000. The programme involves an in-depth study of concepts in both theoretical and experimental Physics. It provides students a scope of developing their problem-solving, mathematical, communication skills and critical thinking which further broadens into interpreting scientific data that is essential for scientific research.

About ISPA

Indian SpectroPhysics Association (ISPA) is a brain child of Veteran Professor and Scientist Ariviyal Mudumunaivar Sethu Gunasekaran. ISPA was started on April 23, 1998, it is a registered society under whose auspices, conferences, workshops and seminars are organized. ISPA is the peak of a strong belief that enlightening young minds and empowering them to pursue research through Spectroscopy. ISPA has an enviable record of having organized 16 International conferences and 18 National Conferences. ISPA also has organized 20 State Level Technical Seminars in Physical Sciences for PG and M.Phil. students, since 1999. Indian SpectroPhysics Association (ISPA) finds its place in encouraging renowned and young scientists by honouring them with ISPA Awards in the recognition of the research findings of the scientists. 15 Veteran scientist Awards, 54 Life Time Achievement Awards, 86 ISPA Ariviyal Mudumunaivar Sethu Gunasekaran Awards, Dr. S. Mohan Awards, are given to researchers who have made excellent contributions in the field of Research, during Conferences/ Seminars organized by ISPA. An international consortium has been made with the Medical University of Sofia for a tune of 1000 crore for a research project., Visit www.ispa.org.in for more details.

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Focus of the Conference

The International Conference ICOSMOS 2025 is a pioneering event conveying the current cutting-edge field advancements in nanomaterials, bio-materials, energy storage materials, computational methods and astrophysics. The interdisciplinary conference will bring together leading researchers, academicians and industry experts to discuss innovative ideas and solutions. It is intended to create a good exposure to researchers by interacting with experts in their research fields and also present their research findings and build a network in the proposed theme areas.

Focused Area of the Conference

-Spectroscopy
- Astrophysics
- Crystal Growth
- Crystallography
- Bio Physics
- Medical Physics
- Ceramic Materials
- Drug Design
- Instrumentation
- Luminescent Material
- Solar Technology
- Transport Properties
- Thin Film Technology
- Magnetic Materials

-DFT Analysis
- Materials Science
- Theoretical Physics
- MEMS
- Nanotechnology
- Nonlinear Optics
- Optoelectronic Devices
- Photocatalysts
- Polymer Composites
- Modelling & Simulation
Surface Engineering
- Semiconductor Materials
- Molecular dynamics

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PG Department of Physics

In association with

Indian SpectroPhysics Association (ISPA)
Chennai, India

Invite you to the

International Conference on Spectroscopy, Materials and Observational Sciences (ICOSMOS - 2025)

20th February 2025

In Commemoration Of National Science Day

Time: 9:30 a.m.

Venue : Vidhya Darshan Auditorium, First Floor, MBA Block

Chief Guest

Prof S. Gunasekaran, Ph.D.,D.Sc.,
Founder-President, Indian SpectroPhysics Association
Dean [R&D]
St. Peter's Institute of Higher Education and Research, Avadi, Chennai.

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Dr. S. Muniyappan
Dr. C. Yogeswari

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Dr. Z. Delci
Ms. K. Laavanya

Convenor
Dr. B. Sylaja
Head i/c

Capt. Dr. S. Santhosh Baboo
Principal
Patron, ICOSMOS 2025

Dr. Ashok Kumar Mundhra
Secretary
Chief Patron, ICOSMOS 2025

We Welcome You All!!

Programme Schedule

Inauguration

09: 30 a.m. *Invocation*

09: 35 a.m. *Welcome Address*

Dr. B. Sylaja
Convenor, ICOSMOS 2025

09: 40 a.m. *Focus of the Conference*

Dr. Z. Delci
Organising Secretary, ICOSMOS 2025

09: 45 a.m. *Presidential Address*

Capt. Dr. S. Santhosh Baboo
Patron, ICOSMOS 2025
Principal

09: 55 a.m. *Unveiling the Portrait of Sir CV Raman*

10: 00 a.m. *Inaugural Address*

Prof. S. Gunasekaran, Ph.D., D.Sc.,
Founder-President, ISPA

10: 15 a.m. *Release of Conference Proceedings*

10: 20 a.m. *Conferring ISPA Awards*

ISPA LifeTime RecognitionAward

Prof. Revathy Srinivasan, Ph.D.
Former Professor, SIET College, Chennai
Prof. B. Krishnan, Ph.D.
Former Principal, DDGD Vaishnav College, Chennai

ISPA Ariviyal Mudhumunaivar Sethu. GunasekaranAward

Dr. S. Djodilatchoumy, Ph.D.
Associate Professor & Head, Department of Computer Science,
Chellamal College for Women, Chennai

10: 30 a.m. *Felicitation*

Dr. Bhavana Lalchand, Ph.D.
Postdoctoral Research Fellow, Graduate Institute of Astronomy,
National Central University, Taiwan

10: 35 a.m. *Vote of Thanks*

Ms K. Laavanya
Organizing Secretary, ICOSMOS 2025

10: 40 a.m. *High Tea*

Technical Sessions

Technical Session – I
Chair Person: Dr. K. Annapoorani

11:00 a.m. – 11:40 a.m.

Dr. Bhavana Lalchand, *Ph.D.*
Postdoctoral Research Fellow, Graduate Institute of Astronomy, National Central University, Taiwan
Topic: *Star Cradles: A Perspective on the Formation of Brown Dwarfs in Star-forming Regions*

Technical Session – II
Chair Person: Dr. T. Sivaranjani

11:40 a.m. – 12:20 p.m.

Dr Janani P, *Ph.D.*
Instructional Designer Head (Academics), Echtian Contents Private Limited, Mumbai

Topic: ***Role of Reflectance Spectroscopy for Diagnosing Thyroid Disorders and Assessing the Effectiveness of an Ayurvedic Drug Thyronil in the Treatment of Thyroid***

Technical Session – III
Chair Person: Dr. A. Chinnammal Janaki

12:20 p.m. – 01:00 p.m.

Dr S. Srinivasan, *Ph.D.*
Associate Professor, Department of Physics, Presidency College, Chennai

Topic: ***Simulation and Performance Analysis of Some Solar Cells***

Lunch: 01:00 p.m. – 01:45 p.m.

Oral and Poster Presentation

01:45 p.m. – 03:15 p.m.

Judges:
Oral Presentation: Prof. S. Srinivasan &
Dr. A. Chinnammal Janaki
Poster Presentation: Dr. Bhavana Lalchand & Dr. K. Gomathi

Valedictory Function

03: 30 p.m.	*Invocation*
03: 35 p.m.	*Welcome Address* *Dr. S. Muniyappan* *Joint Organising Secretary, ICOSMOS 2025*
03: 40 p.m.	*Report of the Conference* *Dr. C. Yogeswari* *Joint Organising Secretary, ICOSMOS 2025*
03:45 p.m.	*Presidential Address* *Capt. Dr. S. Santhosh Baboo* *Patron, ICOSMOS 2025* *Principal*
03: 50 p.m.	*Valedictory Address* *Dr. S. Srinivasan,* Ph.D, *Associate Professor, Department of Physics* *Presidency College, Chennai*
03: 50 p.m.	*Address by President ISPA* *Prof. S. Gunasekaran,* Ph.D., D.Sc., *Founder-President, ISPA*
04: 00 p.m.	*Feedback & Distribution of Certificates*
04: 10 p.m.	*Vote of Thanks* *Dr. B. Sylaja* *Convenor, ICOSMOS 2025*
04: 15 p.m.	*National Anthem*

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PREFACE

NOTE FROM THE EDITORIAL COMMITTEE

The International Conference on Spectroscopy, Materials and Observational Sciences (ICOSMOS - 2025) was organized by the PG Department of Physics, Dwaraka Doss Goverdhan Doss Vaishnav College on 20th February 2025. It was our esteem privilege to conduct this conference in association with Indian SpectroPhysics Association (ISPA).

The conference laid an international platform with renowned experts sharing their insights, showcasing innovations and fostering collaborations in diverse thrust areas of scientific knowledge addressing the participants coming from various sectors including academicians, research scholars and postgraduate students. The high standards of the research papers and speakers highlighted the event's success. The conference proceedings included abstracts from speakers, advisory board members, faculty, and external contributors, offering valuable insights into the field.

We would like to express our sincere gratitude to the organizing committee and everybody who have worked very hard to make this conference a reality and success. We would like to express our deepest gratitude to the distinguished keynote speakers, National and International Advisory Boards and sponsors. We would like to acknowledge all of those who supported ICOSMOS 2025.

We express our heartfelt gratitude to all the members who have helped us directly or indirectly in making this conference grand success internationally. We extend our appreciation to all participants and hope the proceedings will benefit readers scientifically and enhance professional interlacing beyond boundaries.

We are extremely elated to publish the abstract proceedings of this conference ICOSMOS-2025.

With our warmest regards
Editorial Committee
ICOSMOS 2025

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Dr. Ashok Kumar Mundhra
Secretary

A note from the Secretary's Desk

"That's one small step for man, one giant leap for mankind." **-. Neil Armstrong**

Dear Faculty and students of the PG Department of Physics,

I am exhilarated to hear about the upcoming conference on "International Conference on Spectroscopy, Materials and Observational Sciences" (ICOSMOS - 2025). This conference is a pioneering event highlighting the current cutting-edge field advancements in science and technology.

I believe this conference will provide a great opportunity for young researchers to gain the latest knowledge and share the current developments in science and technology.

The interdisciplinary conference will bring together leading researchers, academicians and industry experts to discuss innovative ideas and solutions. It provides a gateway for the participants and ensures researchers to generate new ideas in physics and materials science.

I encourage you to participate actively in brainstorming discussions and build new horizons that can lead to meaningful collaboration in multidisciplinary science.

Best wishes for the successful conduct of the conference. !!!

Best regards

Dr. Ashok Kumar Mundhra
Secretary, DDGDVC
SECRETARY
Dwaraka Doss Goverdhan Doss
Vaishnav College
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Dr. S. Santhosh Baboo, M.Sc., Ph.D.,
Principal

A note from the Principal's Desk

***"Imagination is more important than knowledge. Knowledge is limited. Imagination circles the world."* — Albert Einstein**

Dear Faculty and students of the PG Department of Physics,

I extend my heartfelt congratulations to the PG Department of Physics for organizing the "International Conference on Spectroscopy, Materials and Observational Sciences" (ICOSMOS - 2025).

I am sure this conference showcases the department's academic programs and highlights the importance of Spectroscopy, Materials and Observational Sciences.

This conference will be more useful for researchers, students, and academicians working in the field of multifunctional materials.

By bringing together subject experts from various disciplines you have created a strong platform for thought-provoking discussions, knowledge sharing and collaborative problem-solving

I am sure this conference will provide a pathway for the participants to exchange their knowledge and new ideas. Finally, I would like to acknowledge the organizing committee for securing substantial input of research abstracts and creating volumes of knowledge.

I would like to appreciate the team's every step, in bringing this to light and wish them all success.

Best regards

Capt. Dr. S. Santhosh Baboo
Principal

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Dr. B. Sylaja,
Associate Professor & Head i/c
PG Department of Physics

Note from the HOD's desk
"The only source of knowledge is experience" – Albert Einstein

It is my pleasure to inform that the Post Graduate Department of Physics is organizing the "International Conference on Spectroscopy, Materials and Observational Sciences" (ICOSMOS-2025) on 20th February 2025 in association with Indian SpectroPhysics Association (ISPA) to commemorate National Science Day.

Materials have played such a crucial role in the advancement of civilization that we define entire eras by them. As we strive to create materials that are stronger, lighter, more affordable, functional, and sustainable, innovation continues to shape the future of technology and society.

This conference explores the latest advancements in Nanomaterials, Biomaterials, Energy Storage Materials, Computational Methods, and Astrophysics. It serves as an excellent platform for delegates to exchange knowledge, share insights, and discuss cutting-edge innovations and developments in these fields.

The conference proceedings stand as a testament to the collaborative efforts of research scholars and academicians, bringing together brilliant minds in the fields of material science and spectroscopy. **ICOSMOS-2025** offers a prestigious international forum for presenting and discussing the latest research breakthroughs, emerging technologies, and groundbreaking applications, fostering innovation and global scientific exchange.

I extend my heartfelt congratulations to all the participants whose valuable contributions have enriched this publication. Their research highlights and creative insights are a testament to their passion for learning and innovation.

A special appreciation goes to the students for their active involvement and to the dedicated faculty members and editorial team, whose tireless efforts have made this initiative a reality.

I sincerely wish this publication great success and look forward to many more impactful conference proceedings in the future.

B Sylaja

Dr. B. Sylaja
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Former Registrar, Periyar University, Salem
Former Head, Department of Physics, Pachaiyappa's College, Chennai.

E-mail: president@ispa.org
Website: www.ispa.org.in

16.02.2025

Prof. S. Gunasekaran
Dean, Research & Development

PROLOGUE

It is with immense honor and great enthusiasm that I extend my heartfelt wishes to all the distinguished delegates, researchers, and academicians participating in the **International Conference on Spectroscopy, Materials and Observational Sciences (ICOSMOS – 2025)**, organized by the **PG & Research Department of Physics, Dwaraka Doss Govardhan Doss Vaishnav College (Autonomous), Chennai**, in collaboration with the **Indian SpectroPhysics Association (ISPA)**.

Science thrives on collaboration, and this conference stands as a testament to the spirit of inquiry, discovery, and innovation. The **ICOSMOS – 2025** conference brings together brilliant minds across disciplines to engage in profound discussions on **cutting-edge advancements in spectroscopy, materials science, and observational sciences**, aiming to bridge the gap between theoretical research and real-world applications. It is through such gatherings that scientific communities converge to push the boundaries of knowledge, inspire future generations, and open new avenues for interdisciplinary collaborations.

For more than two decades, **ISPA has shared a strong and enduring association with Dwaraka Doss Govardhan Doss Vaishnav College**, fostering academic excellence and research endeavors. This longstanding collaboration has been instrumental in advancing scientific dialogue, enabling young researchers to engage with global experts, and creating a platform for knowledge dissemination at an international level.

At this momentous occasion, I extend my sincere appreciation to the **Chief Patron, Dr. Ashok Kumar Mundhra, Secretary**, for his unwavering support in fostering academic excellence and scientific research. I also express my deep gratitude to the **Patron, Capt. Dr. S. Santhosh Baboo, Principal**, for his visionary leadership and commitment to strengthening research initiatives. My heartfelt acknowledgment goes to the **Convenor, Dr. B. Sylaja, Head** i/c, whose efforts and dedication have been pivotal in organizing this prestigious event. I also commend the **Organizing Secretaries, Dr. Z. Delci and Ms. K. Lanvanya**, along with the entire organizing committee, for their meticulous planning and tireless dedication in ensuring the success of this conference.

Wishing **ICOSMOS – 2025** great success and impactful outcomes for the scientific community.

Dr. S. Gunasekaran
Founder President, ISPA

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Dr.S.Srinivasan, Ph.D

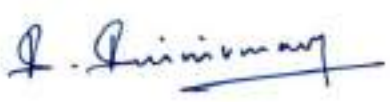
Associate Professor, Department of Physics

Presidency College, Chennai

It gives me immense pleasure that the PostGraduate Department of Physics, Dwaraka Doss Goverdhan Doss Vaishnav College (Shift II) in association with Indian SpectroPhysics Association (ISPA) is organizing an International Conference on Spectroscopy, Materials and Observational Sciences (ICOSMOS-2025) on 20th February 2025 at Dwaraka Doss Goverdhan Doss Vaishnav College (Shift II).

The central theme of the conference is "Spectroscopy, Materials and Observational Sciences". ICOSMOS 2025 provides an opportunity for meeting of International Researchers, Engineers, Scientists and specialists in the various research and development fields of current cutting edge field advancements in materials spectroscopic techniques and astrophysics. The conference offers a premise for global experts to gather and interact intensively on the topics of recent advancements in the field of materials for their various societal applications.

I hope eminent speakers will cover the theme of the conference from different perspectives. I am privileged to say that this conference will definitely offer suitable solutions to the global issues. The success of this Conference is solely on the dedication and efforts of innumerable people who started working on the preparations for almost a year in many ways to make this Conference become a reality. Eventually I express my special thanks and appreciation to all. I wish ICOSMOS 2025 all the best for its success.



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CONTENTS

CONTENTS

INVITED TALKS

ORAL PRESENTATION

POSTER PRESENTATION

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ABSTRACTS OF THE RESOURCE PERSONS

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IT-1

A Light Legendary – Sir CV Raman

Dr. S. Gunasekaran, Ph.D., D.Sc.
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Sir C V Raman

The Great Indian physicist Chandrasekhar Venkata Raman, popularly known as Sir C.V Raman, was born on 7th November, 1888 at Thiruvanaikaval, Trichirapalli district in Tamil Nadu. His father was a physics teacher and so it was natural that Raman developed love for this subject. He was a brilliant student from the very beginning. As a brilliant and promising lad, he passed his matriculation examination at the young age of 12 with 5 years promotion from Madras University. He studied at Hindu College, Visakhapatnam and Presidency College, Madras. He did his M.A. in Physics from the Presidency college and broke all previous records. He obtained his post-graduation degree in Physics in 1907 with the top position. During his student period, he conducted many researches and published his papers in many reputed magazines. His outstanding potential was recognized, and he was given unlimited access to the laboratories, where he pursued investigations of his own design. In November 1906, aged 18, Raman had his first academic paper published. He had initially given it to one of his professors to read, but the professor had not bothered. Raman sent his paper directly to *Philosophical Magazine, London* and it was accepted. Its title was *Unsymmetrical diffraction-bands due to a rectangular aperture*, it was about the behavior of light. Following the publication of his second paper in *Philosophical Magazine*, Raman received a letter from Lord Rayleigh, the eminent British physicist. Rayleigh, unaware that Raman was just a teenage student, sent his letter to "Professor Raman."

Raman saw a 13 years old girl playing a Thyagaraja Keerthana on the Veena. Against all conventions of that time, he arranged his marriage with her. Her name was Lokasundari. In the same year, Raman got the first position in the Financial Service Examination and was appointed as the Assistant Accountant General in Calcutta. There he came in contact with an eminent scientist named Dr. Amritlal Sarkar who was the Secretary of the Indian Association for the Cultivation of Science. This contact with Dr.

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Sarkar proved a turning point in the life of this young scientist. His interest in physics was deep and lasting and so he continued his research work in his spare time in the laboratory of the Association. He published his research results in the leading journals of Calcutta, which were in regard to the subject of propagation of light. These original research papers were of great scientific significance. When these came to the notice of the then Vice -Challenger of Calcutta University, Sir Ashutosh Mukharjee, he appointed him as Professor of Physics in the Calcutta University. During his stay at the University, he continued his research with much more devotion and won immense honour and recognition as a physicist.

He was elected the Fellow of the Royal Society of London in 1924. He discovered the "Raman Effect" in 1928. For it, he was awarded the Nobel Prize for Physics in 1930. He became the first Indian in the Asian countries to win this prestigious honour. With this award, his reputation increased by leaps and bounds and many Universities and institutions of repute honoured him with Ph D and D.Sc. degrees. In December, 1927 he was busy in laboratory when the news came that the well-known physicist A.M. Compton was awarded the Nobel Prize for demonstrating that the nature of X-rays undergoes a change when passed through a matter. This effect came to be known as the "Compton Effect." Encouraged by this discovery, Raman continued his experiments and ultimately proved that light rays can also be scattered. His discovery enabled for the first time, the mapping of possible levels of energy gains of molecules and atoms of a substance and thus discovered their molecules and atomic structure. This discovery of the scattering of light led to the development of a simple alternative to infra-red spectroscopy, namely, Raman Spectroscopy.

Raman Effect happens when molecules of a medium scatter light energy particles known as photons. The spectrum varies with the nature of the transparent medium used to scatter the light. Raman Effect has proved to be of great scientific value and with its help the structure of more than 200 compounds has been known. He also gave us the scientific explanation for the blue colour of the sky and the ocean. He explained that the blue color of the ocean was as a result of the scattering of sunlight by the molecules of the water. He travelled widely abroad delivering lectures about his discoveries and researches. In 1933 he became the Director of the Indian Institute of Sciences, Bangalore. In 1943 he founded the Raman Research Institute at Bangalore. He was knighted in 1927. He was awarded the Bharat Ratna in 1954 and the International Lenin Prize in 1957.

Raman was a born genius and a self-made man and scientist with deep religious convictions. His interests were wide and deep and so were his contributions to the human knowledge and development. Besides optics, he was deeply interested in acoustics—the science and study of sound. His contributions to the mechanical theory of bowed, stringed and other musical instruments like violin, sitar, cello, piano, veena, Tanpura and mridangam have been very significant. He explained in detail how these musical instruments produce harmonious tones and notes. Unfortunately, there is no college or institution to honour Sir CV Raman. He died on November 21, 1970 at the ripe age of 82 at Bangalore and his mortal remains were consigned to flames in the campus of the Raman Research Institute.

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IT-2

Simulation and Performance analysis of Some Perovskite Solar Cell

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Abstract

SCAPS-1D (Solar Cell Capacitance Simulator) is a simulation tool used for modelling solar cells. In this discussion, it was employed to analyse the performance of organic-inorganic halide perovskite solar cells. It solves fundamental semiconductor equations, including Poisson's equation and continuity equations, to evaluate and optimize the performance of solar cells, particularly perovskite structures. Recently, organic–inorganic perovskites showing excellent have manifested great capacity to enhance the performance of photovoltaic systems, owing to their impressive optical and electronic properties. The performance-determining parameters, including the thickness of HTL and AL, as well as the doing and defect density (NA and Nt), were discussed and the performance of the solar cell were evaluated and interpreted.

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IT-3

Role of Reflectance Spectroscopy for Diagnosing Thyroid Disorders and Assessing the Effectiveness of an Ayurvedic Medication in Thyroid Treatment

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Abstract

Fourier transform infrared-attenuated total reflectance (FTIR-ATR) spectroscopy has proven useful in monitoring the efficacy of the Ayurvedic drug Thyronil for treating hypothyroidism in women. This study observed that the lipid-to-protein ratios of hypothyroid patients increased immediately after treatment and then decreased to healthy levels. These ratios can serve as potential biomarkers, suggesting that FTIR-ATR spectroscopy may offer a rapid optical method for continuous monitoring of hypothyroid disorders, making it a valuable tool in personalized medicine.The research also identified ethyl hexadecanoate as the active component responsible for the anti-thyroid properties of Commiphora Mukul (Guggulu) seeds using Gas Chromatography Mass Spectrometry (GCMS). Among the over 190 active components, ethyl hexadecanoate and nine other bioactive compounds showed effective inhibition of lactoperoxidase, a thyroid-related enzyme. The docking scores and glide energies were determined using Schrödinger Maestro software, highlighting ethyl hexadecanoate as the most promising compound with a gliding energy of -33.074 kcal/mol and a docking score of -5.396. The ADME properties of these compounds were analyzed using Qikprop software, confirming their biological activity within acceptable ranges. This study suggests that ethyl hexadecanoate acts against thyroid disorders by blocking lactoperoxidase (LPO) and can be further developed into a potent Ayurvedic drug, Thyronil, for anti-thyroid treatment. Additionally, ongoing research is exploring the use of nanoparticles to enhance the delivery and efficacy of Thyronil and other identified phytochemicals. Nanoparticles can improve bioavailability and targeted delivery, potentially increasing therapeutic effects while reducing side effects. This innovative approach merges modern nanotechnology with traditional medicine, offering promising advancements in the treatment of thyroid disorders. The interdisciplinary research could lead to new developments in both nanomedicine and Ayurvedic drug formulations, providing more effective treatments for thyroid-related health issues.

Keywords: *Ayurveda; Thyronil; Ethyl hexadecanoate; Thyroid.*

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IT-4

Star Cradles: A Perspective on the formation of brown dwarfs in star-forming regions

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Abstract

Brown dwarfs, with masses < 0.08 M_{sun}, fill in the gap in mass between low-mass stars and giant planets. Brown dwarfs and planet-mass objects, having no sustainable nuclear fusion reactions, are relatively bright and warm at birth, thereby readily detectable in star-forming regions or young clusters. These substellar objects are also vital tracers of star formation versus planet formation and serve as key analogues to exoplanets around stars. We have applied the technique of on-off imaging of the 1.45 μm H_2O absorption band seen in typical spectra from late M to L, T, and Y-type objects to identify the substellar population in Perseus cloud complex and other star-forming regions such as Rho Ophiuchi, Orion, respectively. The 1.45 μm imaging together with J and H photometry renders a reliable way to select water-bearing objects relatively free of reddening. We use complementary from WISE, 2MASS, and Pan-STARRS data to identify young stars with dusty circumstellar disks and Gaia EDR3 for parallax and kinematics. My research also focused on the earliest stage of star formation, including how stars gain their masses by accretion from surrounding gas and dust, to measure the accretion variability of protostars. We used the data obtained from the James Clerk Maxwell Telescope/SCUBA-2 Transient Survey of protostars in nearby star-forming regions. This survey is the first dedicated survey for submillimeter variability and complements other transient surveys at optical and near-IR wavelengths, which are not sensitive to the accretion variability of deeply embedded protostars. I will also give a few ideas/suggestions based on my experience of how to follow your passion/dream to pursue a degree in astronomy or any field.

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ABSTRACTS OF PARTCIPANTS

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ORAL PRESENTATION

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OP-1
Third order Nonlinear Optical properties of 4-Chloroaniline derivative Crystal for Photonic Applications

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Abstract

Nonlinear optical (NLO) materials play a major role in photonics, including optical information processing, sensor protector applications, data storage, etc. Some organic compounds exhibit large NLO responses, in many cases, orders of magnitude larger than widely known inorganic materials. A novel crystal derivative of 4-chloroaniline was synthesized using a slow evaporation method. The single and powder X-ray diffraction studies confirm its crystalline structure. UV-Vis-NIR spectroscopy provided linear optical properties. The third-order nonlinear optical (NLO) properties of the grown crystal were probed using the Z-scan technique. The exceptional third-order NLO performance makes this crystal a promising candidate for photonic applications.

Keywords: *Slow Evaporation, XRD, UV-vis-NIR, and NLO.*

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OP-2
Sustainable Solutions: HB-TiO_2 Nanoparticles for Enhanced Photocatalytic Degradation of organic pollutants

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Abstract

Novel HB-TiO_2 nanoparticles were successfully synthesized using the Greens route method and used as photocatalyst with Fenton reagent to degrade pharmaceutical pollutants, specifically paracetamol (PARA), diclofenac (DCF), and tetracycline (TC). The synthesized HB-TiO_2 were characterized using P-XRD, FTIR, UV-Visible DRS, FE-SEM, EDX, DLS and Zeta potential. Using PARA, DCF, and TC as a model pollutant, degradation tests were conducted for various light sources to assess the activation of HB-TiO_2 with the Fenton reagent. The outcomes showed maximum degradation of the model pollutant, reaching a 100% degradation efficiency within 20 minutes. It was proposed that HB-TiO_2 – Fenton reagent activation leads to the breakdown of contaminants. The degradation patterns of pollutants using several approaches, including Fenton's reagent, photocatalyst (HB-TiO_2), photo Fenton catalyst and hydrogen peroxide were also examined. When compared to other methods, it demonstrates that Fenton's reagent, which contains a HB-TiO_2 photocatalyst, has the maximum activity for breaking down pollutants. These results highlight effectiveness as a catalyst in the breakdown of organic pollutants and highlight its potential applications in environmental remediation.

Keywords: *Nano-photocatalytic, Advance Oxidation Processes, TiO_2, Green synthesis, Environmental sustainability*

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OP-3
Synthesis and characterization of La_2FeNdO_6 compound

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Abstract

The double perovskite compound La_2FeNdO_6 has been synthesized by solid-state reaction method, which facilitates the formation of a complex structure combining lanthanides and transition metal ions with oxygen. Structural characterization using X-ray diffraction (XRD) confirmed the orthorhombic crystalline symmetry of the compound, typical for perovskite-related materials. The material's optical properties were examined by UV-Vis Diffuse Reflectance Spectroscopy (DRS), which revealed that La_2FeNdO_6 exhibits semiconductor behavior, with an energy band gap suitable for optoelectronic applications. Additionally, scanning electron microscopy (SEM) analysis was performed to investigate the surface morphology, providing valuable insights into its texture and uniformity. These findings suggest that La_2FeNdO_6 holds significant potential for various advanced applications, including magnetic materials, solid-state lasers, and optoelectronic devices, where its unique combination of electronic, magnetic, and structural properties could be effectively utilized.

Keywords: *Double Perovskite, Solid-state reaction, XRD, UV DRS, SEM.*

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OP-4
Synthesis And Characterization Of Calcium Stabilized Zirconia Nanoparticles

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Abstract

Calcium stabilized zirconia nanoparticles has been prepared using the sol gel method to improve the mechanical and thermal properties. Calcium stabilized zirconia NPs has been synthesized by mixing Zirconium oxychloride solution and calcium oxide solution. NaOH acts as catalyst and it has been used to obtain the required PH(~10). Power X-ray diffraction (XRD) has been used for phase identification, crystallite size analysis, and monitoring phase stabilization. Calcium stabilized zirconia shows suppressed monoclinic peaks because of the incorporation of Ca^{2+} ions into the ZrO_2 lattice, which stabilizes the high-temperature tetragonal/cubic phases at room temperature. Crystallite size has been determined using the Scherrer equation. The synthesized Calcium-stabilized zirconia has found making the materials stronger, more conductive and more sustainable. The conductivity has been found to be increased for Calcium-stabilized zirconia NPs compared with Zirconia. Calcium-stabilized zirconia has applications in fuel cells and refractories. It has high-temperature applications such a molten metal handling and casting. It set to play a key role in clean energy and advanced manufacturing, and next-gen technology.

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OP-5
Green synthesis of ZnO Nanoparticle using leaf extract and their antibacterial and antifungal activities

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Abstract

Nanotechnology deals with creation of material, devices and systems in the nanometer scale. Nanoparticles have many applications in science and technology, including electronics, medicine, agriculture, and more. Zinc oxide nanoparticles (ZnO) are used in an increasing number of industrial products such as rubber, paint, coating, and cosmetics. ZnO has a slew of unique chemical and physical properties, high chemical stability, high electrochemical coupling coefficient, broad range of radiation absorption and high photo stability, which make it among all metal oxides a key technological material and confer upon it its wide applications in varied fields. Green synthesized ZnOs were fabricated biologically using Leucas aspera leaf extract without adding additional chemical precipitating agents. FTIR studies confirmed the functional group present in the green synthesized ZnO nanoparticle.The morphology of the green synthesized ZnO particles was characterized by Scanning Electron Microscopy. The Powder XRD pattern confirmed the structure of green synthesized ZnO. Using Debye Scherer's formula, the crystallite is calculated as 36nm. The ZnO nanoparticle exhibited efficient antibacterial and antifungal activity. It showed good inhibition zone against Staphylococcus aureus and Trichoderma viride. The obtained results confirmed that the green synthesized ZnO nanoparticle seems to be an effective antimicrobial activity.

Keywords : *Green synthesis Nanoparticle, Antimicrobial Study, XRD, SEM.*

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OP-6
Synthesis and Characterization of CMC-PVA-NaCl Hybrid Polymer Electrolytes for Energy Storage Applications

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Abstract

This study focuses on the synthesis of hybrid polymer electrolytes by blending Carboxymethyl Cellulose (CMC) and Polyvinyl Alcohol (PVA) with varying concentrations of NaCl using the casting technique. The structural, ionic conductivity, and electrochemical properties of the prepared samples were analyzed using X-ray Diffraction (XRD), Fourier Transform Infrared (FTIR) Spectroscopy, and Electrical Impedance Spectroscopy (EIS). The results indicate that the highest ionic conductivity at room temperature was achieved at a NaCl concentration of 20 wt.%, which also exhibited the lowest crystallinity percentage. FTIR analysis and IR-deconvolution confirmed that ionic conductivity is strongly influenced by ionic mobility and diffusion coefficient. Electrochemical analysis through Linear Sweep Voltammetry (LSV) demonstrated that the highest conducting sample exhibited significant electrochemical stability. To further evaluate its application potential, the optimized polymer electrolyte was fabricated into an Electrical Double Layer Capacitor (EDLC). The findings suggest that the CMC-PVA-NaCl hybrid polymer electrolyte possesses excellent ionic conductivity and electrochemical stability, making it a promising candidate for energy storage applications, particularly in EDLCs.

Keywords: *Hybrid Polymer Electrolytes, Carboxymethyl Cellulose, Polyvinyl Alcohol, NaCl, Ionic Conductivity, Electrochemical Stability, Electrical Double Layer Capacitor (EDLC).*

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OP-7
Synthesis of ZnO nanoparticles using *Murraya koenigii* and study of their antibacterial & antifungal properties

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Abstract

As a branch of material science, nanotechnology is a research hotspot because of its potential for innovative medical applications. Metal Oxide Nanoparticles (MONPs) developed using green synthesis is now enjoying prominence for diverse uses. To meet current needs, various preparation strategies have been devised to synthesize MONPs. In this perspective, a variety of plant species, algae, isolates of bacteria, microbes, and other organisms have been used as resources for the green chemical route of MONPs synthesis for sustainable development. *Murraya koenigii*, which is part of the Rutaceae family, are commonly referred to as curry leaves. In addition to being a source of calcium, *Murraya koenigii* consist of iron, vitamin C, vitamin A, vitamins B and B2. It has been used extensively in Indian cooking for millennia and has a variety of uses in traditional medicine. Raw green leaves are consumed to treat vomiting, diarrhoea, and dysentery. Additionally, leaves and roots have long been used as bitter, anthelmintic, analgesic, to treat blood problems, leucoderma, piles, inflammation, and itching. In our studies ZnO nanoparticles were successfully synthesized using *Murraya koenigii* by Greens route method and used to study their antibacterial and antifungal properties. The synthesized ZnO were characterized using P-XRD, FTIR, UV-Visible, FE-SEM, EDX, and DLS.

Keywords: *ZnO, Green synthesis, Environmental sustainability, Antibacterial, Antifungal*

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OP-8

Synthesis of ZnO nanoparticles using Clitoria ternatea and study of their antibacterial & antifungal properties

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Abstract

The quality of human life has been significantly enhanced by plants and herbs for millions of years. Green synthesis using plants and plant extracts is favored over other microorganisms due to its safe synthesis without any harmful residues, convenient processing, and ability to facilitate large-scale production. Additionally, plant components and extracts from various portions are used as natural capping and reducing agents. Butterfly pea, or Asian pigeonwings or *Clitoria ternatea*, is a long-used traditional medicinal herb that is a member of the Fabaceae family. Earlier reports showed that the extract of *Clitoria ternatea* flowers have been identified to contain significant levels of calcium, magnesium, potassium, zinc, sodium, and iron. In comparison to other medical floral components, *Clitoria ternatea* flowers have been found to have adequate amount of anthocyanin pigments and strong antioxidant qualities. The flowers are used to treat neurological problems, diabetes, and cardiovascular diseases because of their antibacterial, antiviral, and anti-inflammatory qualities. In our studies ZnO nanoparticles were successfully synthesized using *Clitoria ternatea* by Greens route method and used to study their antibacterial and antifungal properties. The synthesized ZnO were characterized using P-XRD, FTIR, UV-Visible, FE-SEM, EDX, and DLS.

Keywords: *ZnO, Green synthesis, Environmental sustainability, Antibacterial, Antifungal*

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OP-9

Quantum Chemical Computational, Molecular Docking Analysis and Topological Studies of the Ziprasidone.

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Abstract

As one of the deadliest cancers worldwide, liver cancer highlights the urgent need for better treatments. To evaluate the medicinal chemicals' specificity and anti-cancer efficacy in Ziprasidone, a thorough investigation was conducted using density functional theory (DFT) quantum calculations and molecular docking experiments. Molecular stability and reactivity against liver cancer are measured using Ziprasidone global reactivity descriptors. The chemical was confirmed using FT-IR and UV-Vis spectrum analysis. The electronic characteristics of Ziprasidone were examined using the DFT/B3LYP/6-311++G(d,p) functional, Gaussian 09 W, Gauss View 6.0, and Chem Craft 1.8 tools, as well as time-dependent density functional theory (TD-DFT) and Veda 04 program for PED values. The MEP surface of the Ziprasidone molecule, HOMO-LUMO analysis, DOS, RDG, ELF, and LOL were the main subjects of the analysis. Anticancer activity, stability, and reactive sites for electrophilic and nucleophilic assaults were all studied. Furthermore, such binding conformations and interaction patterns with significant liver cancer targets are revealed by molecular docking simulations against protein receptor like 8SZL, demonstrating their potential for therapeutic applications. Because they display the majority of the information pertinent to the chemical, including various physical properties, biological activity, and more, in topological indices descriptors through degree-based QSPR analysis, we can observe that indices that are related to the various index give strong connections for the variables.

Keywords*: Ziprasidone, UV-Vis, Molecular Docking, QSPR Analysis Anticancer.*

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OP-10

FTIR, UV, NMR, Quantum Chemical Calculations, and Molecular Docking Investigations of Cellobiose for Drug Delivery in Cancer Therapy

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Abstract

Cellobiose, a disaccharide derived from cellulose, is investigated as a potential drug carrier for targeted cancer therapy through Density Functional Theory (DFT) and molecular docking approaches. The structural and electronic properties of cellobiose and its drug conjugates are optimized using B3LYP/6-311++ (d, p) ensuring molecular stability and accurate charge distribution analysis. HOMO-LUMO energy gap calculations reveal the compound's electronic reactivity, while MEP mapping identifies active binding regions, crucial for drug-target interactions. ELF and LOL analyses provide insights into charge delocalization and bonding characteristics, supporting the compound's suitability for controlled drug release mechanisms. The TD-DFT executed UV-visible spectra were in good agreement with the experimental value, and the FT-IR spectra of each vibrational mode were compared with the theoretical spectra and potential energy distribution PED% carried out. Molecular docking simulations confirm strong binding affinity through hydrogen bonding and π-π stacking interactions, supporting its potential as a tumor-targeting. The electron-hole density distribution is analyzed using Multiwfn, revealing significant charge transfer properties crucial for excitation and interaction mechanisms. These findings establish cellobiose-functionalized drug carriers as efficient, stable, and biocompatible platforms for targeted cancer therapy.

Keywords: *Cellobiose, DFT, HOMO-LUMO, Docking, Cancer Therapy.*

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OP-11
Growth and Characterisation of Organic Non-Linear Optical crystal: 4-Methoxy-2-Nitroaniline

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Abstract

The synthesis and characterization of 4-Methoxy-2-Nitroaniline (4M2NA) crystals were carried out to investigate their structural and nonlinear optical properties. The slow evaporation technique was employed to grow high-quality 4M2NA crystals. The crystalline nature and phase purity were confirmed using Powder X-ray Diffraction (PXRD) analysis, which revealed that the crystal belongs to the centrosymmetric monoclinic space group **C2/c**, with well-matched lattice parameters. Fourier Transform Infrared (FTIR) spectroscopy was performed to identify the functional groups and confirm the molecular structure. To explore the nonlinear optical properties, an open-aperture Z-scan experiment was conducted using a **532 nm Nd:YAG laser** to evaluate the nonlinear absorption behaviour. The results demonstrated Reverse Saturable Absorption (RSA) at an intensity of **2.465×10^{12} W/m^2,** with a calculated nonlinear absorption coefficient of **0.52×10^{-10} m/W**. The optical limiting threshold was observed at **7.52×10^{12} W/m^2,** indicating its potential application as an optical limiter. The strong optical limiting properties of 4M2NA suggest its suitability for laser safety mechanisms and photonic device applications.

Keywords: *optical Limiter, Z-scan, Crystal Growth*

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OP-12
Synthesis and Characterization of ZnO nanoparticle using Cissus Quadrangularis Stem Extract

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Abstract

Nanotechnology offers incredible applications in almost all spheres of life due to which this branch of science has gained popularity and attention swiftly. Green synthesis of nanoparticles (NPs) has attracted the researcher's attention due to its rapid, cost-effective, sustainable and eco-friendly nature. Cissus quadrangularis might have antioxidant, pain-relieving, and anti-inflammatory effects. Current studies were carried out to perform and investigate the green synthesis of ZiO NPs with Cissus quadrangularis stems extract. The NPs were characterized by spectroscopic and microscopic techniques including FTIR, UV, X-ray diffraction (XRD) and SEM. The antibacterial and antifungal potential activities of the synthesized NPs were also examined. XRD patterns revealed the hexagonal wurtzite structure of ZnO NPs and a high degree of crystallinity. The average crystallite size of ZnO NPs was 46 nm. SEM images show that ZnO NPs are platelets structures. The green synthesized ZnO nanoparticles exhibited excellent antimicrobial activity against Candida albicans.

Keywords : *ZnO Nanoparticle, UV, FTIR, SEM.*

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OP-13
Influence of Modifier on Optical Studies of Eu^{3+} doped Aluminoborate glasses for Red LED applications

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Abstract

Eu^{3+} ion-doped amorphous materials are attracting a lot of attention in the current technological landscape because of its potential for solid-state lasers and LEDs in photonic devices. As a result, in this study, we tried to improve the Eu^{3+} ions spectroscopic performance in the suggested glasses. Eu^{3+} doped Aluminoborate glasses doped with different modifiers with chemical composition ($5OB_2O_3+15Al_2O_3+15Ti_2O_3+10P_2O_5+10XCO_3+0.1Eu_2O_3$ [X=Sr, Ba, Ca]) are prepared using the melt quenching technique. Different Characterisation techniques such as FTIR, UV, PL and CIE were adopted to understand the fluorescence nature of the prepared glasses. The FTIR spectra can provide information about molecular vibration or rotation associated with a covalent bond. Infrared spectra exhibit several bands with maxima at 446,481,924,1143 cm^{-1}. These bands are characteristic of bond vibrations of the boron-oxygen networks. From the absorption spectra, the Nephelauxetic ratio is calculated and its covalent behaviour was studied. Excitation spectrum was observed for the prominent emission of Eu^{3+}at 613 nm and suitable excitation wavelength was identified. The characteristics of magnetic and electric dipole transitions observed in luminescence spectra were analysed and the prepared glasses were found ideal for red emission. Further CIE colour chromaticity co-ordinates confirms the prepared glasses are ideal for red-emitting materials.

Keywords: *Glasses, Covalency, Borate, CIE chromaticity diagram, Europium.*

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OP-14

Theoretical and experimental study on Dimethyl 2-methoxyhexane-1,6-dioate compound: Its optimization with DFT and structural and spectroscopic investigation, HOMO-LUMO, MEP, atomic charge, and NBO analysis

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Abstract

This study studies Dimethyl 2-methoxyhexane-1,6-dioate utilizing both theoretical and experimental methods, with an emphasis on its possible medicinal uses. The molecular geometry was optimized using Density Functional Theory (DFT) with the Becke, 3-parameter, Lee-Yang-Parr (B3LYP) technique and the 6-311++G (d, p) basis set. Theoretical computations revealed information about the compound's electronic characteristics, including the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, which indicate its stability and reactivity. Molecular Electrostatic Potential (MEP) maps were created to determine reactive sites and electron density distribution. Vibrational assignments were obtained by comparing experimental and computational FTIR data to validate functional groups and molecular vibrations. Natural Bond Orbital (NBO) theory was used to investigate atomic charge distribution and bonding interactions, and non-covalent interactions were studied further using Reduced Density Gradient (RDG), Electron Localization Function (ELF), and Localized Orbital Locator (LOL) methods, which provided insights into the molecule's stability and electron correlation. Experimental validation was carried out using FTIR, NMR, and UV-Vis spectroscopy, which supported the theoretical conclusions. Molecular docking experiments revealed robust interactions with major therapeutic targets, indicating the compound's potential as a medication candidate. The findings suggest that dimethyl 2-methoxyhexane-1,6-dioate is a good option for medicinal uses. Its chemical characteristics, stability, and interactions with biological targets make it a promising substance for future medication development and biomedical research.

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OP-15
NBO, Molecular Orbital and MESP Analysis of 3-O-Methyl-D-Glucose

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Abstract

Fresh leaf extraction from *Ormocarpum sennoides* was carried out by the soxhlet extraction method. The extract has been subjected to GC-MS study, which revealed the presence of 3-O-methyl-D-glucose in the methanolic extract of *Ormocarpum sennoides.* DFT has been performed using the B3LYP/6-311++G (d,p) level to identify inter-molecular interaction and natural bond orbital (NBO) study. The stability of the molecule has been analyzed using NBO analysis. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecule orbital (LUMO) energy gap have been calculated. The molecular electrostatic potential (MEP) of the molecule were constructed.

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OP-16
Spectroscopic characterization, DFT study, topological, molecular docking, and pharmacological analysis of 2, 5-ditert butyl -4-hydroxybenzoquinone

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Abstract

The antibacterial compound 2,5-ditert butyl -4-hydroxybenzoquinone, a member of p-quinones and benzoquinone has focussed on developing antitumor agents. The study analysis of the structure of this benzoquinone shows antibacterial activity, antitumor potential, and also in drug designs. The GC-MS analytical method authenticates the molecular structure of 2,5-ditert butyl-4-hydrobenzoquinone and discloses the structural characteristics. FT-IR, FT Raman, and UV-Vis spectra have been used to characterize the molecule. DFT methods (Density Functional Theory) employing the B3LYP/6-311++G (d, p) basis set are used to analyze the compound's geometrical optimized structure and vibrational frequencies. The electronic properties of the compound are explored through HOMO-LUMO energy gap calculations, while molecular electrostatic potential (MEP) mapping aids in understanding its reactive sites relevant to medicinal applications. For quantifying the distribution of electron density among the atoms in a molecule, the Mulliken atomic charge is used in common along with the atomic charge calculation. The calculated NBO (Natural Bond Orbital) study of the compound molecule (inter-intra, charge delocalization, and hydrogen bonding) has a significant stable link between the donor and the acceptor. The chemical response between ELF and LOL mapping shows the interactions and chemical relationship between and within the fragments. The Reduced Density Gradient determines areas of interest, including bonding or non-bonding interactions, by analyzing the variation in electron density, providing details about the structure and function of molecules. At last, auto docking is utilized to title the compound's biological activity has been examined and shows the examined compound can serve as an important anticancer preventer.

Keywords: *FT-IR, UV-Vis, NBO, Molecular Docking, and benzoquinone*

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OP-17
Molecular Docking and DFT Analysis of ß-D-Gentiobiose for Anti-Cancer Property

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Abstract

An organic molecule that includes ß-D-Gentiobiose. Antimicrobial, antibacterial, antioxidant, anti-inflammatory, and anticancer characteristics are all possessed by the compound mentioned in the title. FT-IR, UV-Vis, and DFT methods are being used to study the genitobiose molecule for various medicinal applications. Using the 6-311++G (d, p) basis set, the geometrical parameters, HOMO-LUMO, and molecular electrostatic potential (MEP) map are analyzed using the B3LYP approach. The NBO 3.1 tool was used to compute the high stabilization interaction (intra-inter, hydrogen bonding, and charge delocalization) between the donor and acceptor in the 3TMH molecules. When examined using XRD values, the improved geometric structure was shown to be stable for both single and double bonds. The electronic transitions carried out by the TD-DFT technique are n→π* and n→σ*. Veda 04 states that there is good agreement between the theoretical spectra of vibrational assignment with PED % and the observed FT-IR spectrum. The chemical fusion between ELF and projection mapping has been used to explain the interactions between LOL and ELF, as well as the strong attraction, strong repulsion, and weak interaction interactions of the ß-D-Gentiobiose under investigation using Reduced Density Gradient (RDG). The docking of it demonstrated the binding nature of the compound compound and how effective the deug is in the anticancer property.

Keywords: *FT-IR, UV–visible, Topological properties, drug-likeness, Molecular Docking studies*

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OP-18

A Theoretical Approach On The Binding Stability And Molecular Interaction Of An Azo-Ester Based Fluorophore With Human Insulin

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Abstract

Molecular docking approach on the binding studies of an azo-ester based fluorophore with Human Insulin were carried out employing Auto-dock 4.2 Molecular docking methodology.In this study,we employ a theoretical approach to investigate the binding stability and molecular interaction with human insulin. Molecular docking and Molecular dynamics (MD) simulation are utilized to explore the binding affinity, conformational changes, and stability of the complex. Key interaction such as hydrogen bonding , pi-pi stacking, and van der waals forces, are analyzed to elucidate the molecular recognition mechanism. The binding free energy is calculated to assess the stability of the interaction, providing insights into the potential application of the fluorophore in insulin-related biomedical research .Our finding suggest that the azo-ester fluorophore exhibits strong and stable interaction with insulin, indicating its potential as molecular probe for insulin detection and structural studies

Keywords: Perovskite photocatalysts, CO_2 reduction, photocatalytic efficiency, tunable bandgaps, defect engineering, heterostructure, surface modifications, co-catalysts, renewable fuels, carbon capture.

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OP-19
Synthesis and Characterization of Ag decorated iron oxide nanoparticles

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Abstract

Hematite (α-Fe_2O_3) is a widely studied iron oxide due to its abundance, stability, and promising applications in catalysis, energy storage, and environmental remediation. Its narrow bandgap enables visible-light absorption, making it a potential candidate for photocatalytic applications. However, pure α-Fe_2O_3 suffers from limited charge carrier mobility and rapid recombination of photo-generated electron-hole pairs, reducing its photocatalytic efficiency. To enhance its performance, noble metal nanoparticles like Ag are incorporated to improve charge separation and boost photocatalytic activity. In this study, Pure and Ag nanoparticles decorated α-Fe_2O_3 were synthesized. The synthesized materials were characterized for structural, morphological, and optical properties. X-ray diffraction studies confirmed the rhombohedral structure of α-Fe_2O_3 and determined the crystallite sizes. Ultraviolet-visible spectroscopy analysis revealed bandgap energies of pure α-Fe_2O_3 and Ag decorated α-Fe_2O_3. Transmission electron microscopy analyzed the size of Ag nanoparticles and scanning electron microscopy examined the morphology of Ag-decorated α-Fe_2O_3. The synthesized material will be further evaluated for dye degradation studies as a photocatalytic application.

Keywords: *α-Fe_2O_3, XRD analysis, ultraviolet-visible spectroscopy, Transmission electron microscopy, Scanning electron microscopy, photocatalytic application.*

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OP-20
Review of the Power of Semiconductor Materials: Paving the Way for Technological Advancement

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Abstract

The basis of many gadgets that have completely changed the way we live, communicate, and calculate, semiconductor materials are essential to contemporary electronics and technology. This abstract gives a brief introduction to semiconductor materials, examining their basic characteristics, uses, new developments, and history from the 1950s to the present. It also examines the development process of semiconductor materials and the main drivers of their advancement. Beginning with the transistor and diode, the fundamental components of semiconductor electronics, it develops into a wide range of other devices, including sensors, light-emitting diodes (LEDs), solar cells, and integrated circuits (ICs). It is emphasized how crucial semiconductors are to the development of digital computers, communication systems, renewable energy conversion, and sensor technologies. Engineers and researchers have improved power conversion efficiency, decreased energy loss, and produced smaller electronic devices by utilizing materials including silicon, gallium nitride (GaN), and silicon carbide (SiC). The transformative potential of semiconductor materials in forming next-generation technologies is examined in this paper, with a focus on how they can propel sustainable energy solutions, improve performance in high-frequency applications, and pave the way for advances in quantum computing and artificial intelligence. As a key force behind technological advancement in the twenty-first century, semiconductor materials' continuous evolution keeps pushing the envelope of innovation.

Keywords: *Semiconductor material, History, Application, Advancement, Quantum computing.*

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OP-21
Preparation, Characterization and Applications of Bio Glasses – A Review

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Abstract

This review covers the preparation techniques and applications of bioactive glass in bone regeneration. Bioactive glasses are extremely promising materials for the development of bone tissue engineering scaffolds due to their tunable physicochemical properties, which can be precisely modified based on their composition. Bioactive glasses are suitable for bone regeneration due to their ability to increase enzymatic activity and promote cellular proliferation. Recent studies have primarily focused on silicate, borate/borosilicate, and phosphate-based bioactive glasses, resulting in significant advances in this field. Furthermore, metallic glasses have been studied for technological and biomedical applications, particularly bone regeneration. Several trace elements have been incorporated into the glass network to improve their biological and mechanical properties, thereby enhancing bone remodelling and associated angiogenesis. This review seeks to clarify the structure-property relationships governing bioactive glasses, with a focus on hydroxyapatite formation, compositional requirements, and future research directions. Furthermore, advances in metallic and doped bioactive glasses, as well as fabrication techniques, will be thoroughly investigated.

Keywords: *Melt quench, sol-gel, solid state, hydroxyapatite (HA), Stimulated body fluid (SBF), bioactivity, bone regeneration.*

ISBN: 978-93-48505-29-3

OP-22
Photophysical and computational analysis of interaction of azo-ester fluorophore with human insulin

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Abstract

Azo-ester dyes have garnered significant attention due to their versatile photophysical properties and potential applications in biomedical research. In this study, we investigate the interaction between an azo-ester dye and human insulin using a combination of spectroscopic and computational techniques. UV-Vis and fluorescence spectroscopy were employed to analyze the photophysical behaviour of the azo-ester dye in the presence of insulin, revealing significant spectral shifts indicative of molecular interactions. Molecular docking simulations further elucidated the binding affinity and possible interaction sites of the azo-ester with insulin. The results obtained from the emission spectrum and docking study revealed that the binding stability of the complex, primarily driven by hydrogen bonding and hydrophobic interaction, which may influence insulin's structural conformation. These findings provide valuable insights into the potential biomedical application of azo-ester dye in drug delivery and biosensing.

Keywords: *Photophysical, molecular docking, fluorophore, UV-Visible.*

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OP-23
Spectroscopic and quantum computational studies of AU (III) complex derived from 1-boc-4-(4-hydroxy-phenyl)-piperazine

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Abstract

1-boc-4-(4-hydroxy-phenyl)-piperazine and its Gold (III) complex have been studied by DFT and investigated their structural, vibrational, and electronic properties. Structural stability is confirmed by vibrational frequency analysis. NBO analysis provided charge distribution and molecular interactions. The responsiveness of the compounds is evaluated by examining HOMO and LUMO orbitals. The excited state is analyzed using TD-DFT and UV-Vis absorption spectra with various solvents. NLO studies have been carried out on the molecule and its complex. Visualize charge distribution and reactive sites are found by Molecular Electrostatic Potential (MEP) mapping. The non-covalent interactions are known by the Reduced Density Gradient (RDG) method. ADME predictions study the pharmacokinetic behavior of the compound and its complex. The potential of the compounds for use in medicinal chemistry and drug development is thus highlighted by this work.

Keywords: *DFT; FT-IR; NBO; MEP; HOMO-LUMO*

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OP-24
Temperature dependent magnetic studies on mixed spinel ferrite $MgFe_2O_4$

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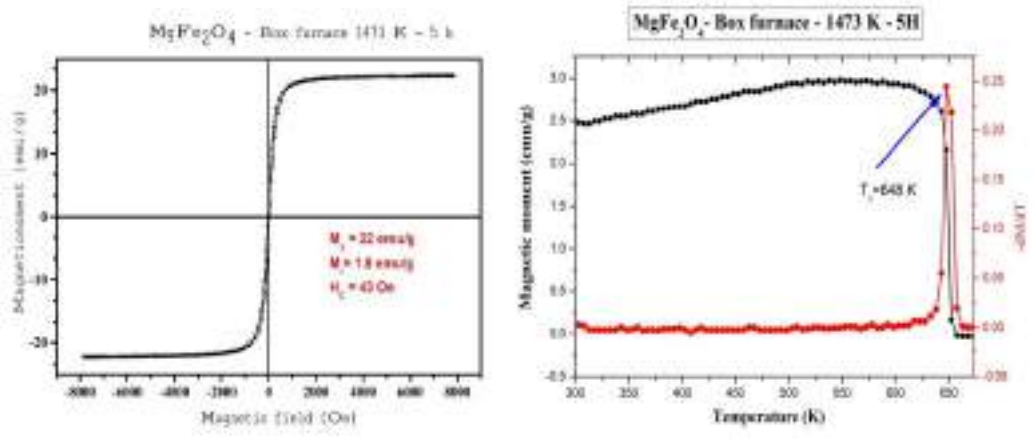
Abstract

Ferrites have been attracting extensive attention due to their application in magnetic storage devices. Among them, Spinel-type ferrites, MFe_2O_4 (M = Mn, Co, Ni, Zn, Mg, Fe, etc.), have gained great interest because of high magnetic permeability and high electrical resistance. This work deals with the preparation of phase pure magnesium spinel ferrite ($MgFe_2O_4$)and study of its structural and magnetic properties. Magnesium ferrite ($MgFe_2O_4$)forms a mixed spinel ferrite with cubic close packed structure. Its Magnetic behaviour is one of the most significant properties which depend on the preparation methods, sintering temperature and grain size. The magnetic studies are done using the vibrating sample magnetometer from which the saturation magnetization, coercivity and retentivity are calculated. Information about the Curie Transition temperature is obtained from the temperature dependent magnetization studies as 648 K.

Keywords: Spinel ferrite, Magnetization, curie temperature



Acknowledgment: *BSK Thank DST Inspire fellow for the award of SRF and Vaishnav Research Promotion Policy- Minor research for their support.*

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OP-25
A Critical Review Of Novel Perovskite-Based Photocatalysts For Co2 Reduction

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Abstract

The growing urgency to combat climate change and lower atmospheric CO_2 levels has driven extensive research into sustainable carbon capture and utilization technologies. Among these, photocatalytic CO_2 reduction using perovskite-based materials stands out due to their adjustable bandgaps, efficient charge carrier mobility, and strong light absorption properties. Compared to traditional semiconductors, perovskite oxides (e.g., $SrTiO_3$, $LaFeO_3$, and $BaTiO_3$) offer high stability, superior charge transport, and effective photocatalytic activity, enabling the conversion of CO_2 into valuable fuels such as CO, CH_4, and methanol. This review explores the latest advancements in the development and modification of perovskite-based photocatalysts for CO_2 reduction, emphasizing their structural, electronic, and catalytic characteristics. Key enhancement strategies, including doping, heterostructure, and surface modifications, are discussed to improve efficiency, selectivity, and long-term stability. Additionally, the role of co-catalysts like noble metals and transition metal oxides in enhancing reaction kinetics and charge separation is examined. The study further highlights the impact of defect engineering, hybrid systems, and interface modifications in increasing CO_2 conversion efficiency and product yield. Despite significant progress, challenges related to material durability, large-scale implementation, and economic feasibility persist. Addressing these issues through innovative material engineering and process optimization is essential for the real-world application of perovskite photocatalysts. This work underscores their potential as next-generation materials for sustainable CO_2 reduction and renewable fuel production, contributing to a cleaner energy future.

Keywords: *Perovskite photocatalysts, CO_2 reduction, photocatalytic efficiency, tunable bandgaps, defect engineering, heterostructure, surface modifications, co-catalysts, renewable fuels, carbon capture.*

ISBN: 978-93-48505-29-3

OP-26
Structural and Spectral Characterization, Vibrational assignments, Molecular Docking and DFT calculations of Pravastatin

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Abstract

The Vibrational spectral studies and the electronic absorption spectrum of Pravastatin were performed using Fourier Transform Infra-Red (FT-IR), UV-Vis and NMR techniques. FT-IR have been recorded and analyzed to identify the presence of functional groups. UV-Vis spectroscopy has been recorded to analyze the absorbance spectra of a title compound in a solid. Calculations of vibrational frequencies of the Anti –lipidemic drug was carried out using Gaussian 09 program package through density functional theory (DFT) approach with B3LYP exchange correlation functional and 6-311G(d,p) basis set. Chemical Stability & Reactivity of Pravastatin have been obtained from frontier molecular orbital (HOMO and LUMO). The Mullikan atomic charges have also been computed. The Natural Bond Orbitals (NBO) analysis was performed to study the stability and charge delocalization of the compound. To understand the nature of the compound ELF and LOL studies has been performed and the Non – covalent interactions were explored using Density Reduced Gradient (RDG) approach. Molecular docking and molecular dynamics have been performed for Pravastatin.

Keywords: *FT-IR Spectroscopy, UV-Vis Spectroscopy, B3LYP, Density functional theory (DFT), Pravastatin.*

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OP-27
Review on Bimetallic Alloy Catalysts for Hydrogen Evolution Reaction

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Abstract

Usage of hydrogen as a fuel is a substantial approach for the environmentally friendly future. To produce large amount of hydrogen in molecular form, water splitting technique is adopted. To reduce the overpotential in hydrogen evolution reaction(HER), electrocatalysts have become inevitable. Among the various catalysts, bimetallic alloys have become the prominent material for HER due to the synergistic effect of alloying. Parameters including reaction kinetics, catalytic activity and stability can be altered by optimizing the alloying process. While alloying, the altering of electronic structure lead to improved hydrogen adsorption capacity resulting in efficient hydrogen evolution. Despite their high efficiency, noble metals(Pt, Rh, Ir) should eventually be replaced by non-noble metals owing to their cost and stability. Transition metals including Nickel(Ni), Cobalt(Co), Tungsten(W) and Molybdenum(Mo) are playing a vital role in HER activity. The valence states of transition elements makes them accessible for adsorption of hydrogen. The tailoring effect while the synthesis of alloy with carbonaceous metals and other frameworks elevates the number of active sites for hydrogen adsorption. Few of the efficient transition alloys and their overpotential for HER from literature are listed in Table 1.

Table 1. List of transition alloys and their overpotential.

Alloy	**Overpotential**
Ni-Mo	86 mV @ 10 mA/cm^2
Ni_1|Co_9/CP	105 mV @ 10 mA/cm^2
Ni–W–P/Mo	75 mV @ 10 mA/cm^2
Ni_1Co_3@NC	28 mV @ 10 mA/cm^2

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OP-28

Experimental and Theoretical spectroscopic (FTIR, UV-Visible,) analysis, natural bonding orbitals and molecular docking studies of 1, 3, 3-trimethyl-2-oxybicyclo [2.2.2] octane (1TOBO) compound

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Abstract

In the current study the title molecules previously been shown to have anticancer properties of few cancers cell line and biological activity of asthma via anti-inflammatory cytokine inhibition. Experimental and computational exploring on the natural bio-molecular structure, electron transition, solute solvent and vibrational characteristics of 1, 3, 3-trimethyl-2-oxybicyclo [2.2.2] octane stimulated by B3LYP/6-311++G (d, p) set and spectral data recorded in the range 400-4000 cm^{-1}. The 1TOBO molecular structure has identified from GC-MS study by extract of Zingiber Officianale Roscoe. NBO elucidates the delocalization of charge due to intermolecular interactions. The vibrational modes of 1TOBO strong correlation among experimental and computational spectral have completed. The UV-Vis spectra of corresponding gas phase and solvent-liquid estimated by TD-SCT process well agreement with reported XRD data. The expended by using Auto dock process to determine the lowest binding impact on the 1TOBO with appropriate cancer-proteins 7QTZ, 1OXR investigated by molecular docking.

Keywords: *DFT, Multi Wave Function, Molecular Docking studies.*

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OP-29
Eco-Friendly Synthesis and Advanced Characterization of ZnO Nanoparticles Using Guggulu Resin

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Abstract

The green synthesis of nanoparticles has emerged as a promising approach due to its environmental sustainability, cost-effectiveness, and minimal toxicity. This study reports the green synthesis of **zinc oxide (ZnO) nanoparticles** using **guggulu resin (Commiphora mukul)** as a natural reducing and stabilizing agent. The bioactive compounds present in guggulu resin, including terpenoids, flavonoids, and phenolic groups, play a dual role in facilitating the reduction of Zn^{2+} ions and stabilizing the resultant nanoparticles, thereby enhancing their colloidal stability.

The synthesized ZnO nanoparticles were subjected to extensive **structural, morphological, and optical characterization**. **Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM)** revealed a **spherical morphology** with a uniform size distribution in the nanometer range. **Dynamic Light Scattering (DLS)** confirmed the nanoscale hydrodynamic diameter and polydispersity index. The presence of functional groups responsible for the stabilization of ZnO nanoparticles was confirmed through **Fourier Transform Infrared Spectroscopy (FTIR)**, which indicated strong interactions between the bio-organic compounds of guggulu resin and the nanoparticle surface. **X-Ray Diffraction (XRD) analysis** verified the **hexagonal wurtzite crystalline structure** with high phase purity. **UV-Visible Spectroscopy** demonstrated a characteristic absorption peak in the ultraviolet region, consistent with the band gap energy of ZnO nanoparticles.

The findings of this study establish guggulu resin as an effective and sustainable bio-template for the green synthesis of ZnO nanoparticles, offering a novel route for **biomedical, catalytic, and environmental applications**. The biocompatibility of these nanoparticles further enhances their potential for **antimicrobial coatings, targeted drug delivery, photocatalytic degradation of pollutants, and advanced electronic materials**, reinforcing the significance of green nanotechnology in sustainable scientific advancements.

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OP-30
Structural and optical property of $ZnTiO_3$ ceramics

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Abstract

The Perovskite has a renewed interest nowadays due to their properties useful for application in gas sensors, ultra violet light emitter and Microwave resonators. Zinc Titanate, ZnTiO3, is a Perovskite having major application in solar cells and microwave detectors. ZnTiO3 has been prepared by High Energy Ball Mill Assisted Sintering Technique. Characterization using X-Ray Diffraction confirms the formation of phase pure $ZnTiO_3$, the structural properties were studied using HR-TEM and the optical property is studied using UV-Visible spectroscopy.

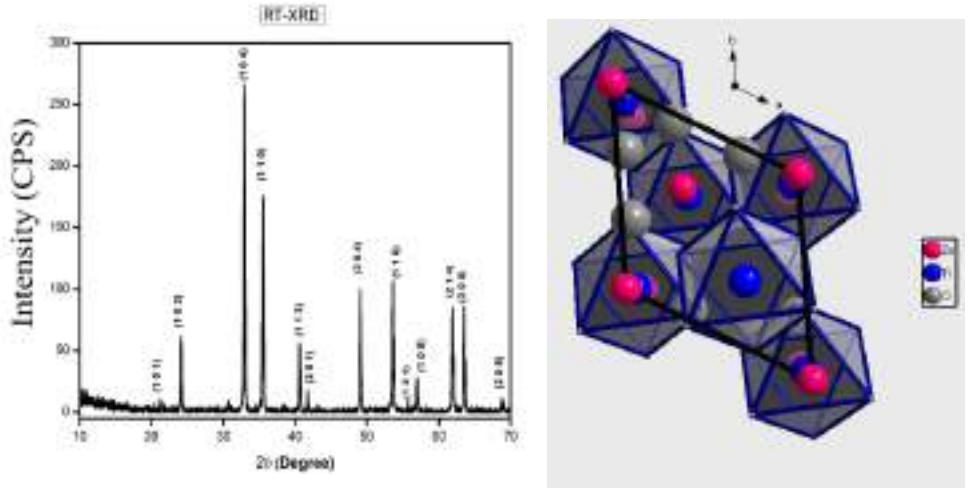

Figure 1: XRD shows the formation of ZnTiO3 and crystal structure of $ZnTiO_3$

Keywords: *Pervoskite, ball milling, Zinc titanate*

Acknowledgment: *BSK Thank DST Inspire fellow for the award of SRF and Vaishnav Research Promotion Policy- Minor research for their support.*

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OP-31
STUDIES ON UROTROPHINE P-NITROPHENOL MONOHYDRATE (UPNM) FOR NLO APPLICATIONS

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Abstract

An organic single crystal Urotrophione p-nitrophenol monohydrate (UPNM) has been grown successfully from an aqueous solution by slow evaporation technique. The single crystal X-ray diffraction shows that UPNM belongs to triclinic crystallographic system with the space group P1. The functional group and vibrational modes of the crystal have been identified using FTIR spectrum. By using UV-vis-NIR spectrum, the cut-off wavelength was found to be around 391 nm and the optical band gap energy was estimated as 3.17 eV. The fluorescence effect of the grown crystal was examined via fluorescence spectroscopy. The crystal's second harmonic generation (SHG) and third-order nonlinear susceptibility were analysed through experimental approaches. The thermal stability of the grown crystal were studied by using TG/DTA thermogram. The results from these investigations collectively provide evidence that the grown UPNM crystal holds non-linear optical applications.

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OP-32
Study on L-Glutaric 4-nitrophenolate (G4NP) Crystal for Nonlinear Optical Applications

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Abstract

Non-linear optical (NLO) single crystals have gained significant attention in recent years due to their ability to perform essential functions such as frequency shifting, optical modulation and optical switching. These single crystals find applications in areas like telecommunication, signal processing, and optical interconnections. Organic L-glutaric 4-nitrophenolate (G4NP) single crystal was grown by slow evaporation solution technique with dimensions approximately 23 × 3 × 2 mm^3. To determine the unit cell parameter, the grown crystal was analyzed using single crystal X-ray diffraction. The XRD studies confirmed that the grown G4NP belongs to monoclinic crystal system with noncentro symmetric space group $P2_1$. The FT-IR spectral analysis was used for identifying the functional groups and bonding nature of the grown crystal. The linear optical behavior was analyzed by UV-vis-NIR spectrum, recorded from 200-1400 nm. The grown G4NP single crystal exhibits a broad transparency band about 65% in the visible to NIR region. The lower cut-off wavelength was found to be 480 nm. The second-harmonic generation efficiency of the G4NP crystal was determined using the powder Kurtz–Perry technique, and it was found to be 2.3 times higher than that of standard potassium dihydrogen phosphate material. The mechanical properties were evaluated using Vickers microhardness.

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OP-33
Hirshfeld Surface, Fukui Function, Molecular docking, Molecular Dynamics Investigation on HIV Organism with 2,6-Dibromo-4-chloroaniline

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Abstract

2,6-Dibromo-4-chloroaniline is a planar molecule. Functional analysis based on vibrational modes is made clearer by spectral analysis. Quantum chemical calculation are characterized, its electronegativity in addition to local characteristics such as electrophilicity and Fukui function. ELF study aims to understand the quantitative behavior of electrons within a system. Docking simulation has been used to assess the energy of binding and coupling between the enhanced protein and ligand combination molecules. The research and development of new drugs heavily relies on the chemical properties of toxicity, metabolism, excretion, distribution, and absorption. The Hirshfeld surface was a helpful tool for illustrating characteristics, such as the electrostatic potential of a molecule inside a crystal structure, that could be quickly and easily learned.

Keywords: *Molvib**,** Fukui Function, Wave function (RDG, ELF, LOL), Hirshfeld Surface, Molecular Docking, Molecular Dynamics, GMX_MMPBSA, ADMET*

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POSTER PRESENTATION

PP-1

Structure Determination of small molecule using single crystal X-Ray Diffraction

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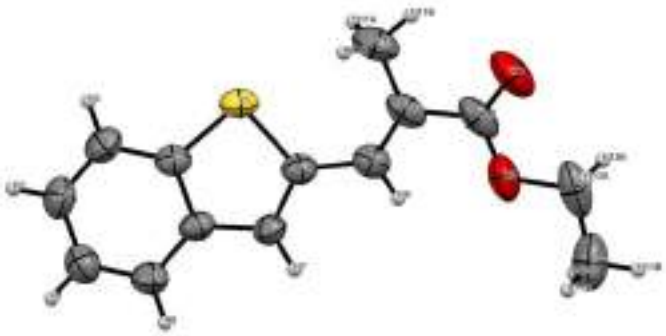
Abstract



THE ORTEP PLOT OF Ethyl(E)-3-(Benzo[B]Thiophen-2-Yl)-2-Methyl Acrylate [$C_{14}H_{14}O_2S$)]
(DISPLACEMENT ELLIPSOIDS ARE DRAWN AT 50% PROBABILITY LEVEL)

Single Crystal X-Ray Diffraction (SCXRD) is a technique used to determine the three-dimensional structure of molecules by analysing the diffraction pattern produced when a single crystal is exposed to X-ray radiation. SHELX (SHELXS & SHELXL) is a software package that is useful for solving and refining single-crystal X- ray diffraction data sets. The crystal structure of the title compound, Ethyl(E)-3-(benzo[b]thiophen-2-yl)-2-methyl acrylate ($C_{14}H_{14}O_2S$), crystallized in the orthorhombic space group Pca21, was solved and refined using Direct methods with an R factor of 0.0602. The Benzothiophene derivatives are found to have diverse biological activities which includes uses in anti-depressants, anti-inflammatory treatments, anti-tumor therapies, estrogen receptor modulators, and anti-fungal agents. Pharmaceutical drugs like Arzoxifene, Brexipiprazole, Raloxifene, and Zileuton utilizes benzo[b]thiophene in their core structure. The acrylate moiety found to act as anti-cancer, anti-oxidant, and anti-inflammatory medicines. In the benzothiophene ring system, the dihedral angle between the fused five and six membered rings is 1.68 (3)° which indicates that the benzothiophene ring system is not exactly planar. The sum of the angles around the atom C8

(359.9°) indicates sp^2 hybridization. However, atom C8 deviates by 0.126 Å from the mean plane through atoms C4, C7 and S1 indicating a slight degree of pyramidalization. The plane of the methyl acrylate unit and the benzothiophene ring system have a dihedral angle of 11.85 (5)° whereas the plane of the benzothiophene ring system and the methyl group forms a dihedral angle of 79.06 (9)° indicating that they are almost perpendicular to each other. The molecular structure is stabilised by weak intramolecular interactions.

Keywords: *Single-Crystal X-ray diffraction, SHELX, Hybridisation, Dihedral angle, Intramolecular interactions.*

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PP-2

Investigation on 3-mercaptopropionic acid capped cadmium sulphide quantum dots for energy applications: Structural, morphological and optical properties

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Abstract

Cadmium sulphide (CdS) quantum dots were synthesized through chemical precipitation technique using 3-mercaptopropionic acid as a capping agent under methanolic medium. Identification of crystal structure of CdS was done through powder X-ray diffraction analysis. Fourier transform infrared analysis revealed the presence of functional groups in the synthesized CdS sample. Scanning electron and transmission electron microscopic analyses revealed the morphology, particle size and crystal structure of CdS quantum dots. Absorption nature of CdS quantum dots was analyzed through UV-vis-NIR diffuse reflectance spectroscopy. Emission property of CdS quantum dots was determined using photoluminescence analysis. The CIE color chromaticity coordinates revealed the dominant emission color of CdS quantum dots. The results of this research work give a better understanding to the suitability of CdS quantum dots to various energy related applications.

Keywords: *Nanoparticles; Quantum dots; Crystal structure; Reflectance; Color chromaticity.*

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PP-3
Synthesis and Characterisation of Copper Oxide Nanoparticles by Precipitation Method

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Abstract

Copper oxide (CuO) nanoparticles have gained significant attention due to their diverse applications in catalysis, sensors, energy storage, and biomedical fields. In this study, CuO nanoparticles were synthesized via a simple and cost-effective precipitation method using copper sulphate ($CuSO_4 \cdot 5H_2O$) and sodium hydroxide (NaOH) as precursors. The synthesized nanoparticles were subjected to comprehensive characterization to evaluate their structural, morphological, optical, thermal, and vibrational properties. Fourier Transform Infrared (FTIR) spectroscopy confirmed the presence of Cu–O stretching vibrations at ~520 cm^{-1} and the absence of organic impurities. Ultraviolet-Visible (UV-Vis) spectroscopy showed a strong absorption peak around 270–320 nm, with an estimated band gap of 2.1 eV, suggesting quantum confinement effects. Thermogravimetric and Differential Thermal Analysis (TG-DTA) indicated good thermal stability with a major weight loss observed around 280°C due to the removal of residual precursors. Fourier Transform Raman (FT-Raman) spectroscopy identified characteristic vibrational modes of CuO at 298, 343, and 632 cm^{-1}, confirming the monoclinic phase. Powder X-ray Diffraction (XRD) analysis confirmed the formation of highly crystalline CuO nanoparticles with a monoclinic structure (JCPDS No. 48-1548), and the average crystallite size was estimated to be ~25 nm using the Scherrer's equation. Scanning Electron Microscopy (SEM) images revealed nearly spherical particles with slight agglomeration, while Transmission Electron Microscopy (TEM) analysis showed nanoparticles with an average size of 20–30 nm and a uniform distribution. The comprehensive characterization of CuO nanoparticles synthesized by the precipitation method demonstrates their potential for various applications in optoelectronics, catalysis, and biomedical fields.

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PP-4
Synthesis And Characterisation Of Zinc Oxide Nanoparticles By Precipitation Method

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Abstract

Zinc oxide (ZnO) nanoparticles have attracted considerable interest due to their wide-ranging applications in optoelectronics, catalysis, sensors, and biomedical fields. In this study, ZnO nanoparticles were synthesized using a simple and cost-effective precipitation method with zinc nitrate ($Zn(NO_3)_2 \cdot 6H_2O$) and sodium hydroxide (NaOH) as precursors. The synthesized nanoparticles were thoroughly characterized to investigate their structural, morphological, optical, thermal, and vibrational properties. Fourier Transform Infrared (FTIR) spectroscopy confirmed the presence of Zn–O stretching vibrations at ~470 cm^{-1}, along with the absence of organic contaminants. Ultraviolet-Visible (UV-Vis) spectroscopy revealed a strong absorption peak around 360 nm, with an estimated optical band gap of ~3.3 eV, demonstrating the semiconducting nature of the material. Thermogravimetric and Differential Thermal Analysis (TG-DTA) showed good thermal stability, with minor weight loss attributed to the removal of adsorbed water and residual precursors. Fourier Transform Raman (FT-Raman) spectroscopy exhibited characteristic ZnO vibrational modes at 330, 440, and 580 cm^{-1}, confirming the hexagonal wurtzite phase. Powder X-ray Diffraction (XRD) analysis validated the formation of highly crystalline ZnO nanoparticles with a hexagonal wurtzite structure (JCPDS No. 36-1451). The average crystallite size, calculated using the Scherrer equation, was found to be ~22 nm. Scanning Electron Microscopy (SEM) images illustrated a spherical morphology with slight agglomeration, while Transmission Electron Microscopy (TEM) analysis provided high-resolution images indicating a particle size range of 15–25 nm with uniform distribution. The comprehensive characterization of ZnO nanoparticles synthesized via the precipitation method highlights their potential for applications in photocatalysis, sensors, and biomedical research.

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PP-5
Synthesis, Characterisation And Anti Microbial Activity Of Magnesium Oxide Nanoparticle

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Abstract

Magnesium oxide nanoparticles are odourless and non-toxic. They possess high hardness, purity and high melting point. MgO NPs appear in a white powder form. They have wide range of applications in catalysis process, biomedical areas and environmental remediation systems. In this study magnesium sulphate has been dissolved in distilled water to get the homogenous solution. The base solution has been prepared by dissolving sodium hydroxide in distilled water. By using dropper the sodium hydroxide solution has been added to magnesium sulphate solution. The investigating sample has been obtained by precipitation. The structural and morphological characteristics of the synthesized MgO nanoparticles were analyzed using X-ray diffraction (XRD). This has been confirmed the formation of cubic-phase MgO with high crystallinity. The antimicrobial activity and antifungal activity of the synthesized MgO MPs reveals that these particles are exhibiting good inhibition against the microbes namely Staphylococcus aureus, Escherichia coli, Candida albicans, Trichoderma viridie.

PP-6

Phytochemical Identification Of Borassus Flabellifer And Biological Evaluation Of Its Anti-Oxidant And Anti-Cancer Activity

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Abstract

Borassus flabellifer, the palmyra palm, is a versatile tree with a rich history of use in various traditional medicine systems, including Ayurveda and Siddha. This rich ethnomedicinal history suggests the presence of bioactive compounds with potential therapeutic properties, making B.flabellifer a subject of ongoing scientific investigation. The phytochemicals have become more popular due to their countless medicinal uses, as they play a vital role against number of diseases such as asthma, digestive issues, arthritis, cancer, etc. The present study was carried out to identify the phytochemicals present in the ethanol extract of the fruit seeds of Borassus flabellifer by Gas Chromatography-Mass Spectrometry (GC-MS) technique which resulted in the identification of twenty-two phytochemicals. The research work investigates the in vitro evaluation of anti-oxidant and anti-cancer properties of the ethanol extract of the fruit seeds of Borassus flabellifer. The antioxidant activity of the fruit seeds of Borassus flabellifer using DPPH assay, demonstrated that a concentration at 1000 µg/ml resulted in 62.57% DPPH inhibition. This indicates a positive correlation between extract concentration and its ability to scavenge free radicals, suggesting the presence of strong antioxidant property. Furthermore, the anti-cancer potential of the fruit seeds of Borassus flabellifer was studied against the MCF-7 breast cancer cell using cell viability assay. The highest concentration at 1000µg/ml exhibited the most substantial reduction in cell viability, with only 24.87% of cells remaining viable control to the untreated control (100% viability). This result indicates that the fruit seeds of Borassus flabellifer extract possesses strong anti-oxidant and anti-cancer properties and may potentially act as an effective drug.

Keywords*: Fruit seeds of Borassus flabellifer extract, GC-MS, Anti-Oxidant, Anti-Cancer activity.*

PP-7

GC-MS Analysis Of Methanolic Extract Of Curcuma Aromatica And Its Biological Property Studies Of Anti-Bacterial, Anti-Fungal, Anti-Diabetic And Anti-Cancer Activity

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Abstract

Curcuma aromatica or wild turmeric is a plant used in traditional medicine having various healthcare benefits. It is one of the oldest herbs which have been identified as an important medicinal plant by the researchers around the world. The phytochemicals have become more popular due to their countless medicinal uses, as they play a vital role against number of diseases such as asthma, digestive issues, arthritis, cancer, etc. The present study was carried out to identify the phytochemicals present in the methanal extract of the Curcuma aromatica (wild turmeric) by Gas Chromatography-Mass Spectrometry (GC-MS) technique. The GC-MS analysis identified the presence of 16 phytochemicals, suggesting a rich source of bioactive compounds. The methanol extract of Curcuma aromatica were then evaluated for their antibacterial, antifungal, antidiabetic and anti-cancer potential. Agar disc diffusion method was employed to show the antibacterial, antifungal activity by estimating the diameter of zone of inhibition. Antidiabetic assay was done to find out the α-AMYLASE and αGLUCOSIDASE inhibition percentage along with its control percentage and was found that concentration and inhibition percentage are directly proportional to each other thereby confirming the antidiabetic property. The research work also evaluated the anticancer activity of curcuma aromatica on MCF-7 cells against breast cancer. The results of the present study suggested that Curcuma aromatica is a promising source of bioactive phytochemicals with potential antibacterial, antifungal, antidiabetic and anti-cancer properties and may potentially act as an effective drug.

Keywords*: Curcuma aromatica extract, GC-MS, Anti-Bacterial, Anti-Fungal, Anti-Diabetic, Anti-cancer activity.*

PP-8

Pyrimidin-2-Amine Glutaric Acid (P2AGA) Co-Crystal for Optical Limiting Application

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Abstract

The co-crystal of pyrimidin-2-amine and propane-1,3-dicarboxylic acid (glutaric acid) (P2AGA) was grown by slow evaporation method. Colourless transparent crystals of P2AGA were formed. The powder X-ray diffraction pattern has been recorded using Panalytical xpert pro X-ray diffractometer with Cu Ka (k = 1.5405 Å) radiation for the title crystal to identify the crystal structure. It is found that P2AGA co-crystal crystallizes in triclinic crystal system with centrosymmetric space group P$\underline{1}$. The most intense peak at (113) shows the crystalline nature of the co-crystal. The functional group of Pyrimidin-2-amine and glutaric acid (P2AGA) co-crystal responding to IR frequency have been identified using FTIR spectroscopy. The grown P2AGA co-crystal FTIR spectrum was taken between wave number 400cm^{-1} to 4000cm^{-1} at room temperature. Intensity dependent nonlinear absorption studies were conducted using open aperture (OA) Z – scan technique with nanosecond Nd:YAG laser of 532nm. P2AGA crystal unveiled Reverse Saturable Absorption nature with intensity of 2.465×10^{12} W/m^2 with nonlinear absorption coefficient value was found to be 0.76×10^{-10} (m/W). The optical limiting properties were also investigated using the OA data and the limiting threshold were found to be less than some of the reported nanomaterials like Te nanowires, Ag_2Te nanowires which made them a guaranteed candidate as optical limiter in many laser safety and optoelectronic devices.

Keywords: *Crystals; Nonlinear optics; Optical limiter*

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PP-9

Design And Implementation Of An Acoustic Levitation System Using Ultrasonic Sensors

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Abstract

Acoustic levitation is a non-contact method that levitates tiny objects using standing ultrasonic waves. This project demonstrates an ultrasonic levitation system employing a single function generator and an external phase-inversion circuit to create stable pressure nodes for levitation. By generating a standing wave, regions of alternating high and low pressure are formed, allowing objects to be levitated at stable points. The system consists of two ultrasonic transducers placed opposite each other. One transducer receives a 40 kHz sine wave directly, while the second receives an externally inverted 40 kHz signal. This setup generates a standing wave, enabling the levitation of lightweight objects. The proper calibration of the frequency and the alignment of sensors is expected to stabilize the conditions of levitation. The major parameters that govern the efficiency and stability of the levitation setup are to be examined in this proposed setup. Upon its success, this technique could potentially be applied in material handling, microgravity simulations, and high accuracy studies of small particles.

Keywords: *Acoustic Levitation, Ultrasonic Sensor, Phase inversion, Function generator, Contactless Material Handling.*

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PP-10

GC-MS, FT-IR and UV-Vis Investigation of Green Synthesized 3-O-Methyl-D-Glucose

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Abstract

Fresh leaf extraction from *Ormocarpum sennoides* was carried out by the soxhlet extraction method. The extract has been subjected to GC-MS study, which revealed the presence of 3-O-methyl-D-glucose in the methanolic extract of *Ormocarpum sennoides*. DFT has been performed using the B3LYP/6-311++G (d,p) level, to obtain electronic and spectroscopic properties. The optimized parameters (bond length and bond angle) of 3-O-methyl-D-glucose molecules are computed using B3LYP/6-311++G(d,p) and compared with XRD data related to the structure. The FT-IR spectra of **3-O-methyl-D-glucose** was recorded in the region 4000–450 cm^{-1}. FT-IR spectra of 3-O-methyl-D-glucose were theoretically obtained using the 6-311++G(d,p) basis set by the DFT method. The vibrational modes were calculated using vibrational energy distribution analysis VEDA 4 program. The UV-Vis spectrum was recorded in the region 400–200 nm.

PP-11
Exoplanet Detection and Characterization Using The Radial Velocity Method

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Abstract

Exoplanets, planets that orbit stars outside our solar system are key to understanding how planetary systems form and whether habitable worlds exist beyond Earth. As of early 2025, over 7,000 exoplanets have been confirmed, with many more waiting to be confirmed. These planets are detected using various methods, including the radial velocity method, transit method, direct imaging, and microlensing. Among these, the radial velocity method is one of the most widely used. This method identifies exoplanets by detecting small movements in a star, called wobbling, caused by the gravitational pull of an orbiting planet. As the star moves slightly toward and away from Earth, its light shifts in wavelength due to the Doppler effect (blueshift when moving closer and redshift when moving away). By analysing these shifts, the presence of a planet can be confirmed, along with details about its orbit, such as period, eccentricity, and minimum mass. This research focuses on analyzing radial velocity data to detect exoplanets, beginning with 51 Pegasi b, the first exoplanet discovered around a Sun-like star. Additionally, synthetic radial velocity curves are generated for hypothetical star-planet systems to investigate how orbital eccentricity influences velocity variations over time. For the real data, the Lomb-Scargle periodogram, a Fourier transform-based method designed for unevenly spaced data, is employed to identify key periodic signals Future work will focus on extracting orbital details using phase-folding methods. This study focuses on a simplified scenario, avoiding complications like multi-planet systems and binary stars. While similar analyses have been done before, the goal is to verify computational techniques by matching results with existing exoplanet catalogues.

Keywords: *Radial velocity method, Doppler effect, Computational techniques, Lomb-Scargle periodogram, Phase-folding, Orbital parameters.*

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PP-12

Investigation on MnO/g-C_3N_4 nanoparticle for Supercapattery application

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Abstract

The rapid expansion of modern electronic devices has created a demand for efficient energy storage and conversion systems with suitable energy and power densities. In this study, we present the hydrothermal synthesis of MnO/g-C_3N_4 nanocomposite materials designed for high-voltage supercapattery applications. The surface morphology and particle size of the synthesized nanocomposite were analysed using SEM. The crystalline structure and planes of the material were examined through powder XRD. FTIR was used to analyse the chemical composition of the synthesized material. The specific capacitance and cycle rate of the nanocomposite were determined through cyclic voltammetry and galvanostatic charge-discharge studies. The specific capacitance of the synthesized electrode was found to be 760 F/g at 1A. The enhanced performance of the device can be attributed to the synergistic effect of both capacitive (non-faradaic) and battery-type (non-capacitive) processes in the charge storage mechanism of the nanocomposite.

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PP-13
Synthesis and Characterization of Zirconia Nanoparticles

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Abstract

Zirconia has been used in dental and orthopaedic implants due to its high strength and biocompatibility. It is also used in refractory materials and fuel cells due to its high thermal stability and ionic conductivity. Zirconia demonstrates exceptional chemical inertness, withstanding exposure to harsh chemicals and environments without degrading or reacting. Pure Zirconia exhibits monoclinic, tetragonal or cubic phases, XRD pattern may vary depending on the specific synthesis method, processing conditions and sample preparation. Zirconia (ZrO2) nanoparticles were synthesized from zirconium oxychloride and NaOH using sol-gel method. Zirconium oxychloride solution has been mixed with NaOH solution to get required PH. NaOH is added as a catalyst to maintain high pH environment. Synthesized Zirconia is kept in the furnace for 10 hours at 500°C. Zirconium oxychloride has been used as a precursor due to its high purity and can produce high yields of Zirconia. Power X-ray diffraction (XRD) has been recorded and used for phase identification, crystallite size analysis, and monitoring phase stabilization. Grain size has been determined. Future perspective includes controlled drug release, exploring novel composite formulation, improving the optical and hardness properties of Zirconia.

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PP-14
Synthesis And Characterisation Of Nickel Oxide Nanoparticles By Precipitation Method

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Abstract

Nickel oxide (NiO) nanoparticles have garnered significant attention due to their applications in catalysis, energy storage, gas sensors, and electronic devices. In this study, NiO nanoparticles were synthesized using a simple and cost-effective precipitation method, utilizing nickel nitrate hexahydrate ($Ni(NO_3)_2 \cdot 6H_2O$) and sodium hydroxide (NaOH) as precursors. The synthesized nanoparticles were subjected to extensive characterization to evaluate their structural, morphological, optical, thermal, and vibrational properties.Fourier Transform Infrared (FTIR) spectroscopy confirmed the formation of Ni–O bonds with a characteristic stretching vibration at ~460 cm^{-1}, while the absence of organic impurities was also verified. Ultraviolet-Visible (UV-Vis) spectroscopy exhibited a broad absorption peak around 350–380 nm, corresponding to an estimated optical band gap of ~3.5 eV. Thermogravimetric and Differential Thermal Analysis (TG-DTA) revealed the thermal stability of the nanoparticles, with a major weight loss occurring around 300°C due to the decomposition of residual precursors. Fourier Transform Raman (FT-Raman) spectroscopy identified distinct vibrational modes at 500 and 720 cm^{-1}, confirming the NiO phase.Powder X-ray Diffraction (XRD) analysis validated the formation of a highly crystalline cubic NiO structure (JCPDS No. 47-1049), with an estimated average crystallite size of ~20 nm, as calculated using the Scherrer equation. Scanning Electron Microscopy (SEM) images revealed a nearly spherical morphology with mild agglomeration, whereas Transmission Electron Microscopy (TEM) provided high-resolution images indicating particle sizes ranging from 15 to 25 nm with uniform distribution. The comprehensive characterization of NiO nanoparticles synthesized by the precipitation method suggests their suitability for various technological applications, including catalysis, energy storage, and sensor development.

Keywords: *Nickel Oxide (NiO), Nanoparticles, FTIR Spectroscopy, UV-Vis Spectroscopy, SEM, TEM, XRD*

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